Combinatorial Algorithms for Multidimensional Necklaces

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Abstract

A necklace is an equivalence class of words of length $n$ over an alphabet under the cyclic shift (rotation) operation. As a classical object, there have been many algorithmic results for key operations on necklaces, including counting, generating, ranking, and unranking. This paper generalises the concept of necklaces to the multidimensional setting. We define multidimensional necklaces as an equivalence classes over multidimensional words under the multidimensional cyclic shift operation. Alongside this definition, we generalise several problems from the one dimensional setting to the multidimensional setting for multidimensional necklaces with size $(n_1, n_2, \ldots, n_d)$ over an alphabet of size $q$ including: providing closed form equations for counting the number of necklaces; an $O(n_1 \cdot n_2 \cdot \ldots \cdot n_d)$ time algorithm for transforming some necklace $\tilde{w}$ to the next necklace in the ordering; an $O((n_1 \cdot n_2 \cdot \ldots \cdot n_d)^5)$ time algorithm to rank necklaces (determine the number of necklaces smaller than $\tilde{w}$ in the set of necklaces); an $O((n_1 \cdot n_2 \cdot \ldots \cdot n_d)^6(d+1) \cdot \log d(q))$ time algorithm to unrank multidimensional necklace (determine the $i^{th}$ necklace in the set of necklaces). Our results on counting, ranking, and unranking are further extended to the fixed content setting, where every necklace has the same Parikh vector, in other words every necklace shares the same number of occurrences of each symbol. Finally, we study the $k$-centre problem for necklaces both in the single and multidimensional settings. We provide strong approximation algorithms for solving this problem in both the one dimensional and multidimensional settings.

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1 Introduction

A necklace is an equivalence class of words of a fixed length over a finite alphabet under the cyclic shift (rotation) operation. More specifically an equivalence class of \(n\)-character strings/words over an alphabet of size \(q\) is known as \(q\)-ary necklace of length \(n\) and the class of aperiodic necklaces is known as Lyndon words. In order to represent a necklace (or a Lyndon word) as a single word a string of characters which is lexicographically smallest out of all of its possible rotations is used. Lyndon words and necklaces are fundamental combinatorial objects arising in the field of text algorithms [34], in the construction of single-track Gray codes [53, 55], analysis of circular DNA and splicing systems [11], in the enumeration of irreducible polynomials over finite fields [35], and in the theory of free Lie algebras [2].

Many computational problems have been formulated and studied for fixed length combinatorial necklaces over a finite alphabet including counting the number of necklaces, generating, ranking (computing a rank according to a previously fixed order), and unranking (generation of the \(i\)-th combinatorial object) necklaces. Graham, Knuth and Patashnik provide equations for counting both the number of necklaces and Lyndon words (aperiodic necklaces) in [21]. The first algorithms for generating necklaces were designed by Fredricksen and Kessler [15], and Fredricksen and Maiorana [14], which were later proven to run in constant amortised time (CAT) by Ruskey, Savage and Wang [50]. Cattell, Ruskey, Sawada, Serra, and Miers provided a further CAT algorithm for the generation of necklaces and Lyndon words [6].

The existence of polynomial time ranking and unranking algorithms for necklaces (cyclic words) remained an open problem for many years and has been only recently solved. The first class of cyclic words to be ranked were Lyndon words by Kociumaka, Radoszewski, and Rytter [34] who provided an \(O(n^3)\) time algorithm, where \(n\) is the length of the word. An algorithm for ranking necklaces was given by Kopparty, Kumar, and Saks [35], without tight bounds on the complexity. An \(O(n^2)\) time algorithm for ranking necklaces was provided by Sawada and Williams [54]. More recently, the open problem of ranking \(q\)-ary bracelets of length \(n\) (the equivalence class of words under the combination of the rotation and reflections), posed by Sawada and Williams, was solved in \(O(q^2 \cdot n^4)\) time in [1].

Algorithms for multidimensional combinatorial necklaces has remained a largely unexplored area in combinatorics on words [39, 57]. A multidimensional necklace is an equivalence class of multidimensional words under translational symmetry, which is the natural generalisation of the shift operation in 1D, see Figure 1. This work aims to fill the gap by developing a set of efficient combinatorial algorithms for multidimensional necklaces.

![Figure 1: An illustration of translational symmetry for a 3 x 3 word. Note that all four words can be reached from one another through two-dimensional translation denoted \((g_1, g_2)\).](image)

Two-dimensional necklaces have been recently studied with the motivation of counting the number of toroidal codes in [4] and can be used in the construction of two dimensional Gray codes [5]. However the most direct application of multidimensional necklaces up to dimension three is the combinatorial representation of crystal structures. In computational chemistry, crystals are represented by periodic motives (or coloured tessellations) known as “unit cells”. Informally, translational symmetry can be thought of as the equivalence of two crystals under translation in space. This intuitively make sense in the context of real structures, where two different “snapshots” of a unit cell both represent the same periodic and infinite global structure. When discrete unit cells are represented by layers, then

![Figure 2: The crystal of \(SrTiO_3\) (left) and its 3D (middle) and 1D (right) necklace representations.](image)

they directly correspond to classical combinatorial necklaces (cyclic words), see [10]. Alternatively, 3D
representations of unit cells are 3-dimensional necklaces, see [9]. Figure 2 provides an illustration of the relationship between crystals and necklaces for both 1 and multiple dimensions, showing how the unit cell of SrTiO₃ can be represented as a necklace of size 2 × 2 × 2 over an alphabet with four letters (blue, green, red, grey); there is one ion of strontium (green cubelet), one ion of titanium (blue cubelet), three ions of oxygen (red cubelets), and three empty (grey) cubelets. Moreover, recent work [13] has even shown the need for representing structures that are not only periodic in three spacial dimensions, but also in the fourth dimension of time. The algorithms for multidimensional necklaces can replace currently used random generation [10] of unit cells leading to potentially identical crystal structures in the process of configuration space exploration.

The paper generalises many results and provides efficient solutions for several problems on q-ary d-dimensional necklaces of size \( n = (n_1, n_2, \ldots, n_d) \). Most notably:

- closed form formulas for the number of necklaces, Lyndon words, and atranslational necklaces
- linear time (relative to the necklace size) algorithm for generating next multidimensional necklaces
- \( O(N^d) \) time algorithm for ranking a d-dimensional necklace, where \( N = \prod_{i=1}^{d} n_i \)
- \( O\left( N^{d+1} \cdot \log^d(q) \right) \) time unranking algorithms for generating the \( i \)th necklace in \( N_q^d \)
- \( O(N^{2k}) \) time approximation algorithm with approximation factor of \( 1 + \frac{\log_q (kN)}{N - \log_q (kN)} \)

for \( k \) center selection on necklaces based on the overlap distance function.

Beyond classical necklaces we also look at fixed-content necklaces. A set of necklaces has fixed content if every necklace in the set has the same Parikh vector [42]. As with general necklaces, there have been results for counting [19], and generating [33, 51] both fixed content necklaces and bracelets.

The set of proposed algorithms for dimensions two and three is a strong contribution to field as it fills a gap in the literature and has direct real-life applications in the context building algorithmic foundation for analysis of crystal structures. Moreover we feel that natural generalisation to any dimension strengthens the paper overall providing universal tools for building efficient algorithms on necklaces of any size.

## 2 Preliminaries

Let \( \Sigma \) be a finite alphabet. For the remainder of this work we assume \( \Sigma \) to be made of symbols corresponding to the set \( \{1, 2, 3, \ldots, q\} \), ordered such that \( 1 < 2 < 3 < \ldots < q \), and by extension \( q = |\Sigma| \). We denote by \( \Sigma^* \) the set of all words over \( \Sigma \) and by \( \Sigma^n \) the set of all words of length \( n \). The notation \( \bar{w} \) is used to clearly denote that the variable \( \bar{w} \) is a word. The length of a word \( \bar{w} \in \Sigma^* \) is denoted \( |\bar{w}| \).

We use \( \bar{w}_i \), for any \( i \in \{1, \ldots, |\bar{w}|\} \) to denote the \( i \)th symbol of \( \bar{w} \). Given two words \( \bar{w}, \bar{u} \in \Sigma^* \), the concatenation operation is denoted \( \bar{w} : \bar{u} \), returning the word of length \( |\bar{w}| + |\bar{u}| \) where \( (\bar{w} : \bar{u})_i = \bar{w}_i \) if \( i \leq |\bar{w}| \) or \( \bar{u}_{i-|\bar{w}|} \) if \( i > |\bar{w}| \). Given a word \( \bar{w} \), the Parikh vector of \( \bar{w} \), denoted \( P(\bar{w}) \) is a \( q \) length vector such that \( P(\bar{w})_i \) contains the number of times that the \( i \)th symbol of \( \Sigma \) appears in \( \bar{w} \).

Let \( [n] \) return the ordered set of integers from 1 to \( n \) inclusive. More generally, let \( [i, j] \) return the ordered set of integers from \( i \) to \( j \) inclusive. Given 2 words \( \bar{u}, \bar{v} \in \Sigma^* \), \( \bar{v} \) is lexicographically smaller than \( \bar{u} \) if there exists an \( i \in [||\bar{u}||] \) such that \( \bar{u}_i \bar{u}_{i+1} \ldots \bar{u}_{i+|\bar{v}|} = \bar{v}_{i+1} \bar{v}_{i+2} \ldots \bar{v}_{i+|\bar{v}|} \) and \( \bar{u}_i < \bar{v}_i \). For a given set of words \( S \), the rank of \( \bar{v} \) with respect to \( S \) is the number of words in \( S \) that are smaller than \( \bar{v} \).

The translation of a word \( \bar{w} = \bar{w}_1 \bar{w}_2 \ldots \bar{w}_n \) by \( r \in [n-1] \) returns the word \( \bar{w}_{r+1} \ldots \bar{w}_n : \bar{w}_1 \ldots \bar{w}_r \), and is denoted by \( \langle \bar{w} \rangle_r \), i.e. \( \langle \bar{w}_1 \bar{w}_2 \ldots \bar{w}_n \rangle_r = \bar{w}_{r+1} \ldots \bar{w}_n \bar{w}_1 \ldots \bar{w}_r \). Under the translation operation, \( \bar{u} \) is equivalent to \( \bar{v} \) if \( \bar{v} = \langle \bar{u} \rangle_r \), for some \( r \). The \( t \)th power of a word \( \bar{w} = \bar{w}_1 \ldots \bar{w}_n \), denoted \( \bar{w}^t \), equals \( \bar{w} \) repeated \( t \) times. A word \( \bar{w} \) is periodic if there is some word \( \bar{u} \) and integer \( t \geq 2 \) such that \( \bar{w}^t = \bar{w} \). A word is aperriodic if it is not periodic. The period of a word \( \bar{w} \) is the aperriodic word \( \bar{u} \) such that \( \bar{w} = \bar{u}^t \).

A necklace is the equivalence class of words under the translation operation. A word \( \bar{w} \) is written as \( \bar{w} \) when treated as a necklace. Given a necklace \( \bar{w} \), the canonical representation of \( \bar{w} \) is the lexicographically smallest element of the set of words in the equivalence class \( \bar{w} \). The canonical representation of \( \bar{w} \) is denoted \( \langle \bar{w} \rangle \), and the \( t \)th shift of the canonical representation is denoted \( \langle \bar{w} \rangle_t \). Given a word \( \bar{w} \), \( \langle \bar{w} \rangle \) denotes the canonical representation of the necklace containing \( \bar{w} \), i.e. the representative of \( \bar{u} \) where
The set of necklaces of length \( n \) over an alphabet of size \( q \) is denoted \( \mathcal{N}_q^n \), the size of which is given by \( |\mathcal{N}_q^n| \). Let \( \bar{w} \in \mathcal{N}_q^n \) denote that the word \( \bar{w} \) is the canonical representation of some necklace \( \bar{w} \in \mathcal{N}_q^n \). An aperiodic necklace, known as a Lyndon word, is a necklace representing the equivalence class of some aperiodic word. The set of Lyndon words of length \( n \) over an alphabet of size \( q \) is denoted \( L_q^n \). A necklace \( \bar{w} \) has fixed content for some given Parikh vector \( \Psi \) if \( \Psi(\bar{w}) = \Psi \). The set of fixed content necklaces for some vector \( \Psi \) is denoted by \( L_{\Psi}^d \), and the set of fixed content Lyndon words by \( L_{\Psi}^d \).

The subword of a word \( \bar{w} \) denoted \( \bar{w}[i,j] \) is the word \( \bar{u} \) of length \( |\bar{w}| + j - i - 1 \mod |\bar{w}| \) such that \( \bar{u}_n = \bar{w}_{n-i+a} \mod |\bar{w}| \). For notation \( \bar{u} \subset \bar{w} \) denotes that \( \bar{u} \) is a subword of \( \bar{w} \). Further, \( \bar{u} \subset \subseteq \bar{w} \) denotes that \( \bar{u} \) is a subword of \( \bar{w} \) of length \( i \). If \( \bar{w} = \bar{u} : \bar{v} \), then \( \bar{u} \) is a prefix and \( \bar{v} \) is a suffix.

As both necklaces and Lyndon words are classical objects, there are many fundamental results regarding each objects. The first results for these objects were equations determining the number of necklaces or Lyndon words of a given length. The number of necklaces is given by the equation \( |\mathcal{N}_q^n| = \frac{1}{n} \sum_{d \mid n} \phi(\frac{n}{d}) q^d \) where \( \phi(n) \) is Euler’s totient function. Similarly the number of Lyndon words is given with the equation \( |L_q^n| = \sum_{d \mid n} \mu(\frac{n}{d}) \mathcal{N}_q^d \), where \( \mu(x) \) is the Möbius function. A proof of these equations is provided in [21].

The problem of generating every necklace in the set \( \mathcal{N}_q^n \) for any \( n, q \in \mathbb{N} \) in lexicographic order was solved first by Fredricksen and Maiorana [13]. This algorithm was shown to run in constant amortised time (CAT) in [50]. A more direct CAT generation algorithm was introduced in [6].

Recently the dual problems of ranking and unranking necklaces have been studied. The rank of a word \( \bar{w} \) in the set of necklaces \( \mathcal{N}_q^n \) is in this work defined as the number of necklaces with a canonical representation smaller than \( \bar{w} \). The unranking process is effectively the reverse of this. Given an integer \( i \in [|\mathcal{N}_q^n|] \), the goal of the unranking process for \( i \) is to determine the necklace \( \mathcal{N}_q^n \) with a rank of \( i \).

Lyndon words were first ranked by Kociumaka, Radziszewski, and Rytter [23] without tight complexity bounds. The first algorithm to rank necklaces was given by Kopparty, Kumar, and Saks [35], also without tight bounds on the complexity. A quadratic time algorithm for ranking both Lyndon necklaces was provided by Sawada and Williams [51], who also provided a cubic time unranking algorithm.

In order to establish multidimensional necklaces, notation for multidimensional words must first be introduced. A \( d \)-dimensional word over \( \Sigma \) is an array of size \( \bar{n} = (n_1, n_2, \ldots, n_d) \) of elements from \( \Sigma \). In this work we tacitly assume that \( n_1 \leq n_2 \leq \ldots \leq n_d \) unless otherwise stated. Let \( |\bar{w}| \) be the size of \( \bar{w} \). Given a size vector \( \bar{n} = (n_1, n_2, \ldots, n_d) \), \( \Sigma^{\bar{n}} \) is used to denote the set of all words of size \( \bar{n} \) over \( \Sigma \). For notation, given a vector \( \bar{n} = (n_1, n_2, \ldots, n_d) \) where every \( n_i \geq 0 \), \( \bar{w} \) is used to denote the set \( \{(x_1, x_2, \ldots, x_d) \in \Sigma^d \mid x_i \leq n_i \} \). Similarly \( [\bar{w}]_{\bar{n}} \) is used to denote the set \( \{(x_1, x_2, \ldots, x_d) \in \Sigma^d \mid x_i \leq n_i \} \).

For a \( d \)-dimensional word \( \bar{w} \), the notation \( \bar{w}[p_1, p_2, \ldots, p_d] \) is used to refer to the symbol at position \( (p_1, p_2, \ldots, p_d) \) in the array. Given 2 \( d \)-dimensional words \( \bar{w}, \bar{u} \) such that \( |\bar{w}| = (n_1, n_2, \ldots, n_d-1, a) \) and \( |\bar{u}| = (n_1, n_2, \ldots, n_d, b) \), the concatenation \( \bar{w} : \bar{u} \) is performed along the last coordinate, returning the word \( \bar{v} \) of size \( (n_1, n_2, \ldots, n_d, a+b) \) such that \( \bar{v}[i,j] = \bar{u}[i,j] \mod p_d \leq a \) and \( \bar{v}[i,j] = \bar{u}[i,j] \mod p_d > a \).

For example given the words \( \bar{w} = \begin{bmatrix} a & a & a & b \\ a & a & b & a \end{bmatrix} \) and \( \bar{u} = \begin{bmatrix} b & b & b & b \\ b & b & b & a \end{bmatrix} \).

A multidimensional cyclic subword of \( \bar{w} \) of size \( \bar{n} \) is denoted \( \bar{v} \subset \bar{w} \). As in the 1D case, a subword is defined by a starting position in the original word and set of size defining the size of the subword. The subword \( \bar{v} \subset \bar{w} \) starting at position \( \bar{p} \) with size \( \bar{n} \) is the word \( \bar{v} \) such that \( \bar{v}[i] = \bar{w}[\bar{p}+i] \mod \bar{n} \) for all \( i \). The \( i \)th slice of \( \bar{w} \), denoted by \( \bar{w}_i \), is the subword of size \( (n_1, n_2, \ldots, n_d-1, 1) \) starting at position \( (i, \ldots, 1, 1) \) of \( \bar{w} \). In the 2D case, \( \bar{u}[i,j] \) is used to denote the \( \bar{v}[i,j] \) to denote \( \bar{v}[i,j] = \bar{w}_{i,j} \). A prefix of length \( l \) for a multidimensional word \( \bar{w} \) is the first \( l \) slices of \( \bar{w} \) in order. A suffix of length \( l \) for a multidimensional word \( \bar{w} \) is the last \( l \) slices of \( \bar{w} \) in order.

A \( d \)-dimensional translation \( r \) is defined by a vector \( (r_1, r_2, \ldots, r_d) \). The translation of the word \( \bar{w} \in \Sigma^{\bar{n}} \) by \( r \), denoted \( \langle \bar{w} \rangle_r \), returns the word \( \bar{v} \in \Sigma^{\bar{n}} \) such that \( \bar{v}[i,j] = \bar{w}[\bar{p} + r] \mod \bar{n} \) for all \( \bar{p} \in [\bar{n}] \) where \( \bar{p} = (p_1 + r_1 \mod n_1, p_2 + r_2 \mod n_2, \ldots, p_d + r_d \mod n_d) \). It is assumed that \( r_i \in \{0, n_i - 1\} \), so the set of translations is equivalent to the direct product of the cyclic groups \( \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \ldots \times \mathbb{Z}_{n_d} \). Given two translations \( r = (r_1, r_2, \ldots, r_d) \) and \( t = (t_1, t_2, \ldots, t_d) \) in \( \mathbb{Z}_{n_1} + \mathbb{Z}_{n_2} + \ldots + \mathbb{Z}_{n_d} \). The translation \( (r_1 + t_1 \mod n_1, r_2 + t_2 \mod n_2, \ldots, r_d + t_d \mod n_d) \).

Definition 1. A multidimensional necklace \( \bar{w} \) is an equivalence class of all multidimensional words under the translation operation.
Informally, given a necklace $\bar{w}$ containing the word $\bar{v}$, $\bar{w}$ contains every word $\bar{u}$ where there exists some translation $\bar{v}$ such that $\langle \bar{v}, \bar{r} \rangle = \bar{u}$. Let $N_q$ denote the set of necklaces of size $\bar{v}$ over an alphabet of size $q$.

As in the 1D case, a canonical representation of a multidimensional necklace is defined as the smallest element in the equivalence class, denoted $\langle \bar{w} \rangle$. Similarly, given a word $\bar{v} \in \bar{w}$, $\langle \bar{v} \rangle$ denotes the canonical representation of the necklace $\bar{w}$, i.e. $\langle \bar{v} \rangle = \langle \bar{w} \rangle$. To determine the smallest element in the equivalence class, an ordering needs to be defined. First, we introduce an ordering over translations.

**Definition 2.** Let $Z_{q^n}$ be the direct product of the cyclic groups $Z_{q_1} \times Z_{q_2} \times \ldots \times Z_{q_d}$, i.e. the set of all translations of words of size $\bar{v}$. The translation $g \in Z_{q^n}$ is indexed by the injective function $\langle \bar{w} \rangle \rightarrow \sum_{i=1}^{d} \left( \bar{g}_i \cdot \prod_{j=1}^{i-1} \bar{n}_j \right)$. Given two translations $g, t \in Z_{q^n}$, $g < t$ if and only if $\text{index}(g) < \text{index}(t)$.

Note that $I = (0,0,\ldots,0)$ is the smallest translation and $(n_1 - 1, n_2 - 1, \ldots, n_d - 1)$ is the largest. Further, the translation $(n_1 + i_1, n_2 + i_2, \ldots, n_d + i_d)$ is equivalent to the translation $(i_1, i_2, \ldots, i_d)$. Using this index an ordering on multidimensional words is defined recursively. The key idea is to compare each slice based on the canonical representations. For notation, given two words $\bar{u}, \bar{s} \in \bar{w}$, let $G(\bar{u}, \bar{s})$ return the smallest translation $g$ where $\langle \bar{u} \rangle_g = \bar{s}$.

**Definition 3.** Let $\bar{w}, \bar{u} \in \Sigma^\bar{v}$ and let $i \in [n_d]$ be the smallest index such that $\bar{w}_i \neq \bar{u}_i$. Then $\bar{w} < \bar{u}$ if either $\langle \bar{w}_i \rangle < \langle \bar{u}_i \rangle$, or $\langle \bar{w}_i \rangle = \langle \bar{u}_i \rangle$ and $\text{index}(G(\bar{w}, \langle \bar{w}_i \rangle)) < \text{index}(G(\bar{u}, \langle \bar{u}_i \rangle))$. Further, given necklaces $\bar{w}$ and $\bar{u}$, $\bar{w} < \bar{u}$ if and only if $\langle \bar{w} \rangle < \langle \bar{u} \rangle$.

Note that a 0-dimensional necklace is simply a symbol from $\Sigma$. Hence for 1D necklaces this ordering is equivalent to the lexicographical ordering. An example of the ordering is given in Figure 4. Both $N_q^\bar{v}$ and $\Sigma^\bar{v}$ are assumed to be ordered as in Definition 2. The rank of a necklace $\bar{w} \in N_q^\bar{v}$ is defined as the number of necklaces smaller than $\bar{w}$ in $N_q^\bar{v}$. In the other direction, the $i^{th}$ necklace in $N_q^\bar{v}$ is the necklace $\bar{w} \in N_q^\bar{v}$ with the rank $i$, i.e. the necklace $\bar{w}$ for which there are $i$ smaller necklaces.

$$\bar{w} = \begin{bmatrix} \bar{w}_1 \\ \bar{w}_2 \\ \bar{w}_3 \\ \bar{w}_4 \end{bmatrix} = \begin{bmatrix} a & a & a & b \\ a & a & b & a \\ b & a & a & a \\ b & a & a & a \end{bmatrix}, \quad \bar{u} = \begin{bmatrix} \bar{u}_1 \\ \bar{u}_2 \\ \bar{u}_3 \\ \bar{u}_4 \end{bmatrix} = \begin{bmatrix} a & a & a & b \\ a & b & a & a \\ b & a & a & a \\ b & a & a & a \end{bmatrix}, \quad \bar{v} = \begin{bmatrix} \bar{v}_1 \\ \bar{v}_2 \\ \bar{v}_3 \\ \bar{v}_4 \end{bmatrix} = \begin{bmatrix} a & a & a & b \\ a & b & a & a \\ a & a & b & a \\ b & a & a & a \end{bmatrix}$$

Figure 4: An example of three words, $\bar{w}, \bar{u}$, and $\bar{v}$, ordered as follows $\bar{w} < \bar{u} < \bar{v}$. Note that $\bar{w}_1 : \bar{w}_2 = \bar{v}_1 : \bar{v}_2 = \bar{u}_1 : \bar{u}_2$. However, $\langle \bar{w}_1 \rangle = \langle \bar{u}_3 \rangle = aaab$, which is smaller than $\langle \bar{v}_3 \rangle = aabb$. Further, $\bar{w}_3 < \bar{u}_3$ as $G(\bar{w}_3, \langle \bar{w}_3 \rangle) = 1$ and $G(\bar{u}_3, \langle \bar{u}_3 \rangle) = 2$, which is larger than 1.

One important concept for multidimensional words is that of the period of a word. Informally the period of $\bar{w}$ of size $\bar{v}$ can be thought of as the smallest subword that can tile $d$-dimensional space equivalently to $\bar{w}$. To define the period of a word, it is easiest to first define the concept of aperiodicity.

**Definition 4.** A word $\bar{w}$ of size $\bar{v}$ is aperiodic if there exists no subword $\bar{\bar{v}} \subseteq \bar{w}$ of size $\bar{v}$ such that $m_i \leq n_i$ for every $i \in [1, d]$, and $\bar{w}_j = \bar{\bar{v}}_j$ where $\bar{\bar{v}}_j = (j_1 \mod m_1, j_2 \mod m_2, \ldots, j_d \mod m_d)$ for every position $\bar{\bar{v}}_j \in N_q^{\bar{v}}$ in $\bar{w}$.

**Definition 5.** The period of a word $\bar{u} \in \Sigma^\bar{v}$, denoted Period($\bar{u}$), is the aperiodic subword $\bar{b} \subseteq \bar{u}$ of size $\bar{v}$ such that $\bar{b}_{\bar{i}} = \bar{b}_{\bar{i}}$ for every position $\bar{i} \in [\bar{n}]$ and $\bar{i} = (i_1 \mod m_1, i_2 \mod m_2, \ldots, i_d \mod m_d)$.
Necklaces

Necklaces

Necklaces

Atranslational

Necklaces

Lyndon Words

Necklaces

Lyndon Words

Atranslational

Necklaces

Lyndon Words

Atranslational

Figure 5: Visual representation of the relationships between Necklaces, Lyndon words and atranslational necklaces, namely that $A_q^\pi \subseteq L_q^\pi \subseteq \Lambda_q^\pi$.

By Definition 5 every word, including aperiodic ones, has a unique period \[16\]. In the case of an aperiodic word \(\bar{w}\), the period is simply \(\bar{w}\). A multidimensional necklace \(\bar{w}\) is aperiodic if every word \(\bar{v} \in \bar{w}\) is aperiodic. An aperiodic necklace is called a Lyndon word. The set of Lyndon words of size \(n\) over an alphabet of size \(q\) is denoted \(L_q^\pi\). A related but distinct concept to aperiodic words are atranslational words and necklaces. A word \(\bar{w}\) is atranslational if there exists no translation \(g \neq (n_1,n_2,\ldots,n_d)\) such that \(\bar{w} = (\bar{w})_g\). Equivalently, a necklace \(\bar{w}\) is atranslational if \((\bar{w})\) is atranslational. The set of atranslational necklaces of size \(n\) over an alphabet of size \(q\) is denoted \(A_q^\pi\).

**Definition 6.** A necklace \(\bar{w}\) if size \(n\) is **atranslational** if there exists no pair of translations \(g, h \in \mathbb{Z}_n^\pi\) where \(g \neq h\) and \((\bar{w})_g = (\bar{w})_h\).

In 1D every aperiodic necklace is atranslational, while in any higher dimension every atranslational word is aperiodic, although not every aperiodic word is atranslational. By extension \(A_q^\pi \subseteq L_q^\pi \subseteq \Lambda_q^\pi\).

A visual example of this relationship is given in Figure 5. For example \([a \ b \ a] \) is aperiodic but not atranslational, as there are only two unique representations of the necklace. On the other hand \([a \ a \ b] \) is both atranslational and aperiodic. For notation, \(A\) translates \(\bar{w}\) to \(g\) where \(\bar{w} = \bar{w}_{\bar{u}}\).

**Proposition 1.** Every word \(\bar{w} \in L_q^\pi\) is either in \(A_q^\pi\) or \(\bar{w} = \bar{w}^p : (\bar{w}^p)_g : \ldots : (\bar{w}^p)_{g^{q-1}}\) where:

- \(g\) is a translation where \(g_d = p\) and there exists no translation \(r < g\) where \((\bar{w}^p)^r = \bar{w}^p\).

- \(\bar{u} \in L_q^{\{n_1,\ldots,n_d-1/r,p\}}\), \(t = \frac{r}{p}\) and is the smallest value greater than 0 such that \(g^t = I\).

As in the 1D case, the set of fixed-content multidimensional necklaces is defined. Given a Parikh vector \(\bar{p}\), the set of multidimensional necklaces of size \(n\) with the Parikh vector \(\bar{p}\) is denoted \(N_q^\pi\).

**Definition 7.** The set of necklaces \(N_q^\pi \subseteq N_q^\pi\) contains every necklace \(\bar{w} \in N_q^\pi\) where the Parikh vector of \(\bar{w}\) equals \(\bar{p}\), i.e. \(P(\bar{w}) = \bar{p}\).

As in the unconstrained setting, fixed-content necklaces is further reduced to the set of fixed content Lyndon words, denoted \(L_q^\pi\), and the set of fixed content atranslational necklaces, denoted \(A_q^\pi\).

3 Overview of Results

3.1 Counting

Section 4 provides results regarding counting the number of multidimensional necklaces, Lyndon words, and atranslational necklaces. As well as being important results in their own right, Theorems 1, 2 and 3 provide both closed form formulas to count the cardinality of these sets, along with relationships between the sets. These relationships are particular use for our ranking techniques.

**Theorem 1.** The number of necklaces of size \(n\) over an alphabet of size \(q\) is given by the equation:

\[
|N_q^\pi| = \frac{1}{N} \sum_{f_1|n_1} \phi(f_1) \sum_{f_2|n_2} \phi(f_2) \ldots \sum_{f_d|n_d} \phi(f_d) q^{(N/\gcd(f_1,f_2,\ldots,f_d))}
\]

Where \(N = \prod_{i=1}^d n_i\) and \(\phi(x)\) is Euler’s totient function.
Theorem 1 is derived using the Pólya enumeration formula. This set is used as the basis for our remaining counting equations. Theorem 2 shows how to use the number of necklaces as a subroutine in order to find the number of Lyndon words.

**Theorem 2** The number of Lyndon words of size \( n \) over an alphabet of size \( q \) is given by the equation:

\[
|L_q^n| = \sum_{f_1|n_1} \mu \left( \frac{n_1}{f_1} \right) \sum_{f_2|n_2} \mu \left( \frac{n_2}{f_2} \right) \cdots \sum_{f_d|n_d} \mu \left( \frac{n_d}{f_d} \right) |A_q^{f_1, f_2 \ldots f_d}| 
\]

Where \( \mu(x) \) is the Möbius function.

Theorem 2 is shown by first expressing the number of necklaces in terms of Lyndon words, then inverting the algorithm for generation of 1D necklaces are are translational words. Theorem 2 is derived using the Pólya enumeration formula. This set is used as the basis for our remaining counting equations. Theorem 2 shows how to use the number of necklaces as a subroutine in order to find the number of Lyndon words.

Proposition 1 (in the preliminaries) establishes that the structure of every translational Lyndon word \( w \) is recursively defined as \( \tilde{w} = \tilde{w} : \langle \tilde{w} \rangle_g : \ldots : \langle \tilde{w} \rangle_g^{t-1} \) where \( \tilde{w} \) is a Lyndon word, and \( g \) is the smallest translation such that \( \tilde{w} = \langle \tilde{w} \rangle_g \). For example the translational Lyndon word \( \langle a \ b \ | \ a | \ a | \ b | a \rangle \) is made by repeating the word \( aab \) along dimension 2 under the translation (1) each time. This leaves the problem of counting the number of possible such translations. To this end, the set \( G(l, \mathbb{N}) \) is introduced as the set of all\( \mathbb{N} \) such that \( g \mathbb{N} \times \) times returns the identity operation, and that \( g \mathbb{N} \) returns some distinct group operation. Note that this corresponds to the number of possible translations that can be used to transform an atranslational word of size \( (n_1, n_2, \ldots, n_{d-1}, l) \) into a necklace of size \( n \). The set \( G(l, \mathbb{N}) \) can be expressed as \( G(l, \mathbb{N}) = \{ x \in Z_{n_1, n_2, \ldots, n_{d-1}} | x \equiv 1 \mod n_i \forall i \in [d-1] \} \) such that \( n_i \equiv 0, \exists i \in [d-1] \) such that \( \forall j \in [\frac{n_i}{d} - 1], x_i^j \mod n_i \neq 0 \}

While \( G(l, \mathbb{N}) \) provides the basis for converting the number of ways of repeating some atranslational word to a translational Lyndon word, it is still necessary to account for translational Lyndon words made using a Lyndon word as a basis. The functions \( I(i, l, \mathbb{N}) \) and \( H(i, l, \mathbb{N}, d) \) are introduced as means to count the number of combinations of translations that can be used to transform some atranslational word of size \( (n_1, n_2, \ldots, n_{i-1}, l) \) into a translational Lyndon word of size \( n \).

**Theorem 3** The number of atranslational words of size \( n \) over an alphabet of size \( q \) is given by:

\[
|A_q^n| = |L_q^n| - \sum_{i \in [d]} \sum_{l=1}^{q-1} \left( \begin{array}{l} l - 1 \\ i \end{array} \right) \prod_{r=1}^{l-1} (-\mu \left( \frac{n_r}{d} \right)) |A_q^{n_1, n_2, \ldots, n_{i-1}, l}| \cdot H(i, l, \mathbb{N}, d) \quad 1 < l < n_d
\]

### 3.2 Generation

Section 3 covers the problems of generating necklaces. String generation in lexicographic order is easy. We find the last character which is not equal to \( q \) (the largest symbol in the alphabet \( \Sigma \)) and increase it by 1. Similar methods can be used for the generation of necklaces, such as the classical generation with clock algorithm by Fredricksen and Maiorana [14]. The key tool used by both our algorithm and the algorithm for generation of 1D necklaces are prenecklaces. Formally, a prenecklace of size \( n \) is a word of size \( n = (n_1, n_2, \ldots, n_{d-1}, n_d) \) that is the prefix of the canonical form of some necklace of size \( (n_1, n_2, \ldots, n_{d-1}, n_d) \) for some arbitrary \( m \in \mathbb{N} \). In other words, a word \( \tilde{w} \in \Sigma^n \) is a prenecklace
of size \( \tilde{n} \) if and only if there exists some integer \( m \in \mathbb{N} \) and necklace \( \tilde{v} \in \Lambda_q^{n_1,n_2,...,n_{d-1},n_d+m} \) where \( \langle (\tilde{v}) \rangle_{[1,n_d]} = \tilde{w} \). For example, the word \( ababa \) is a prenecklace of size \( \langle 5 \rangle \), as it can be extended by concatenating the symbol \( b \) to the end, giving the word \( ababab \) which is the canonical representative of the corresponding necklace class. However, the word \( abaa \) is not a prenecklace as \( ab : \tilde{w} : ab < abaa : \tilde{w} \) for every \( \tilde{w} \in \Sigma^+ \). Note that the canonical form of every necklace is itself a prenecklace.

![Figure 6: Example of the generation algorithm being used to move from one necklace to the next, via an intermediary prenecklace.](image)

The main idea behind our algorithm is to generate the set of all prenecklaces of size \( \pi \) over the alphabet \( \Sigma \) in order. By extension, this process generates each necklace in order. The notation \( \mathcal{P}_q^\pi \) is used for the set of all prenecklaces of size \( \pi \) over an alphabet of size \( q \). Given a word \( \tilde{w} \in \mathcal{P}_q^\pi \), our algorithm generates the word \( \bar{u} \) that is subsequent to \( \tilde{w} \) in the ordering. This is done as follows. Starting with \( \bar{w} \), the largest index \( i \) such that \( \bar{w}_i \neq Q \) is determined, where \( Q \) is the word of size \( (n_1,n_2,...,n_{d-1}) \) where every position in \( Q \) is filled with the largest symbol \( q \in \Sigma \). The word \( \tilde{u} \) is created from \( \bar{w} \) by first incrementing the value of the \( i \)th slice of \( \bar{w} \). The incrimination of \( \bar{w}_i \) is done by either translating \( \bar{w}_i \), if \( \bar{w}_i \) has not already been translated as much as possible without returning to the canonical form \( \langle \bar{w}_i \rangle \), or by setting \( \bar{u}_i \) to \( \text{NextNecklace}(\langle \bar{w}_i \rangle) \) if no such translation exists. After incrementing slice \( i \), the remainder of \( \bar{u} \) is made by repeating the first \( i \) slices. Formally, \( \bar{u}_j = \bar{u}_j \mod i \) for every \( j \in [i+1,n_q] \). A high level overview of this process is shown in Figure 6. It is shown that \( \bar{u} \) is a necklace if and only if \( n_d \mod i \equiv 0 \). Repeating prenecklace generation at most \( n_d \) times guarantees that a necklace is generated.

**Theorem 4.** Let \( \bar{w} \) be a word of size \( \pi \). \( \text{NextNecklace}(\bar{w}) \) returns the smallest word \( \bar{u} > \bar{w} \) such that \( \bar{u} = \langle \bar{u} \rangle \) in \( O(N) \) time.

Theorem 4 is proven by first showing that our algorithm generates every prenecklace in order. This is shown in a combinatorial manner, by first providing a key characterisation of prenecklaces, then showing how to generate the subsequent prenecklace from a given prenecklace. This generation process works in a recursive manner, with each prenecklace of size \( \pi \) requiring a \( d-1 \) necklace of size \( (n_1,n_2,...,n_{d-1}) \) to be generated. From this characterisation, the efficiency of the generation algorithm is shown by proving that to generate the next necklace of size \( \pi \), a total of \( n_d \) prenecklaces of size \( \pi \) must be generated. The complexity comes from the recursive process. Each prenecklace requires a necklace of size \( (n_1,n_2,...,n_{d-1}) \) to be generated, in turn requiring \( n_{d-1} \) prenecklaces of size \( (n_1,n_2,...,n_{d-2}) \) to be generated. Repeating this recursive process yields a total of \( N \) operations to generate the next necklace.

### 3.3 Ranking

Section 3 provides our algorithm for ranking multidimensional necklaces. Recall that the rank of a word \( \bar{w} \) within the set of necklaces \( \mathcal{N}_q^\pi \) is the number of necklaces in \( \mathcal{N}_q^\pi \) that are smaller than \( \bar{w} \). At a high level, our ranking algorithm operates by transforming the number of words belonging to a necklace class with a canonical representation smaller than \( \bar{w} \) into the rank of \( \bar{w} \) within the set of necklaces. This transformation is performed via the rank within the sets of atranslational and Lyndon words. Our ranking algorithm is split between a set of theoretical tools, and a set of computational tools. The theoretical tools establish a relationship between the number of such words and the rank of \( \bar{w} \). This motivates our computational tools that are focused on counting the number of such words.

**Theoretical Tools.** For notation \( T(\bar{w}, \bar{f}) \) is used to denote the set of words \( \bar{v} \in \Sigma^+ \) where the canonical representation of the necklace class including \( \bar{v} \) is smaller than \( \bar{w} \), i.e. \( T(\bar{w}, \bar{f}) = \{ \bar{v} \in \Sigma^+, \langle \bar{v} \rangle < \langle \bar{w} \rangle \} \). Our main computational challenge is in computing the size of \( T(\bar{w}, \bar{f}) \) as a black box for the moment, it is shown how to compute the rank of \( \bar{w} \) from the size of \( T(\bar{w}, \bar{f}) \) through two auxiliary classes of sets, the sets of aperiodic words of size \( \bar{f} \in [\bar{f}] \) belonging to a necklace smaller than \( \bar{w} \) denoted \( L(\bar{w}, \bar{f}) \), and the sets of atranslational words of size \( \bar{f} \in [\bar{f}] \) belonging to a necklace smaller than \( \bar{w} \) denoted \( A(\bar{w}, \bar{f}) \). The sizes of \( L(\bar{w}, \bar{f}) \) and \( A(\bar{w}, \bar{f}) \) are determined using the same relationships established by our counting formulae in Section 4. In terms of this notation:

\[ T(\bar{w}, \bar{f}) = L(\bar{w}, \bar{f}) \cup A(\bar{w}, \bar{f}) \]
\[ |L(\bar{w}, \mathbf{m})| = \sum_{f_1|n_1} \mu \left( \frac{n_1}{f_1} \right) \sum_{f_2|n_2} \mu \left( \frac{n_2}{f_2} \right) \cdots \sum_{f_d|n_d} \mu \left( \frac{n_d}{f_d} \right) |T(\bar{w}, \mathbf{f})| \]

\[ |A(\bar{w}, \mathbf{m})| = |L(\bar{w}, \mathbf{m})| - \sum_{i \in \{d \setminus n_i \}} \sum_{\ell = n_i} \left( \frac{\ell - 1}{\ell} \mu(n_i) \right) (-\mu(\frac{n_i}{\ell})) |A(\bar{w}, n_1, \ldots, n_{i-1}, l)| \cdot H(i, l, \mathbf{f}, \mathbf{d}) \quad l < n_i \]

Here \( \mu(n) \) is the Möbius function. Note that computing the sizes of \( L(\bar{w}, \mathbf{m}) \) and \( A(\bar{w}, \mathbf{m}) \) requires computing the size of \( T(\bar{w}, \mathbf{f}) \) to be computed for every \( \mathbf{f} \) where \( n_i \) mod \( f_i \equiv 0 \). By observing that every translational necklace in \( \mathcal{A}_q^T \) corresponds to \( n_1, n_2, \ldots, n_d \) words in \( \mathcal{A}_q^T \), the rank of \( \bar{w} \) within \( \mathcal{A}_q^T \) can be computed by dividing the size of \( A(\bar{w}, \mathbf{m}) \) by \( n_1, n_2, \ldots, n_d \). For notation let \( RA(\bar{w}, \mathbf{f}) \) be the rank of \( \bar{w} \) within the set \( \mathcal{A}_q^T \), \( RL(\bar{w}, \mathbf{f}) \) be the rank of \( \bar{w} \) within the set \( \mathcal{L}_q^T \), and \( RN(\bar{w}, \mathbf{f}) \) be the rank of \( \bar{w} \) within the set \( \mathcal{N}_q^T \). Using the above observation, \( RA(\bar{w}, \mathbf{f}) \) is given by the equation \( RA(\bar{w}, \mathbf{f}) = \sum_{j=1}^{f_1} j \cdot \mathbb{1}(j < j_1) \).

Computing \( RN(\bar{w}, \mathbf{f}) \) using \( RL(\bar{w}, \mathbf{f}) \) and \( RA(\bar{w}, \mathbf{f}) \) is conceptually the reverse of the process for computing the size of \( |A(\bar{w}, \mathbf{m})| \) from using the sizes of \( L(\bar{w}, \mathbf{f}) \) and \( T(\bar{w}, \mathbf{f}) \). Before showing how to transform \( RA(\bar{w}, \mathbf{f}) \) to \( RL(\bar{w}, \mathbf{f}) \), two helper functions are needed for the cases that \( \bar{w} \) is a translational, aperiodic word, i.e. \( \bar{w} \in \mathcal{A}_q^T, \bar{w} \notin \mathcal{A}_q^T \). Let \( g \in \mathcal{Z}_T \) be the smallest translation such that \( \bar{w} = \langle \bar{v} \rangle_g \) and let \( \bar{u} \in \mathcal{A}_q^T \) be the translational period of \( \bar{w} \). As the rank of \( \bar{w} \) within the set \( \mathcal{A}_q^T \) does not count the word \( \bar{u} \), it is necessary to account for the possible translational words with a translational period of \( \bar{u} \), using translations that are smaller than \( g \). The function \( S(g, l, \mathbf{m}) \) returns the number of translations in \( G(l, \mathbf{m}) \) that are smaller than \( g \). In the case that there exists some index \( i \in [d] \) such that \( g_i > 1 \) and \( g_i = 1 \) for every \( i \in [1, d] \) the number of possible translations corresponds to the sum of \( S(r_j, l_j, (n_1, n_2, \ldots, n_j)) \) for \( j \in [1, d] \) where \( l_i = g_i \) and \( l_d = 1 \) for every \( j > i \), and \( r_j \in G(l_j, (n_1, n_2, \ldots, n_j)) \) is the smallest such translation for which \( \bar{w} = \langle \bar{v} \rangle_{r_j} \). For notational convince, the function \( U(\bar{w}) \) is defined as:

\[ U(\bar{w}) = \begin{cases} 0 & \text{if } \bar{w} \text{ is either aperiodic or temporal} \\ \sum_{j=1}^{d} S(r_j, l, (n_1, n_2, \ldots, n_j)) & \text{if } j = i \\ \sum_{j=1}^{d} S(r_j, l, (n_1, n_2, \ldots, n_j)) & \text{if } j > i \end{cases} \]

The rank \( \bar{w} \) within the set \( \mathcal{L}_q^T \) can be expressed as the sum of \( RA(\bar{w}, \mathbf{m}), U(\bar{w}) \) and \( C(\bar{w}, \mathbf{m}) \), where

\[ C(\bar{w}, \mathbf{m}) = \sum_{i \in [d]} \sum_{l = n_i} \left( \frac{l - 1}{l} \mu(n_i) \right) (-\mu(\frac{n_i}{l})) |RA(\bar{w}, [l, \mathbf{f}], (n_1, n_2, \ldots, n_{i-1}, l))| \cdot H(i, l, \mathbf{f}, \mathbf{d}) \quad 1 < l < n_d \]

The rank \( \bar{w} \) within the set \( \mathcal{N}_q^T \) can be computed by taking the sum over \( \mathcal{L}_q^T \) for every \( \mathbf{f} \) such that for all \( i \in [d] \), \( f_i \) is a factor of \( n_i \). The key observation is that every necklace in \( \mathcal{N}_q^T \) must have a period of size \( \mathbf{f} \) where \( n_i \) mod \( f_i \equiv 0 \) for every \( i \in [d] \). Further, the number of necklaces with a period of size \( \mathbf{f} \) smaller than \( \bar{w} \) is equivalent to \( RL(\bar{w}, \mathbf{f}) \). Therefore, the number of necklaces smaller than \( \bar{w} \) can be computed by summing the number of Lyndon words smaller than \( \bar{w} \) for every such \( \mathbf{f} \). Hence the rank of \( \bar{w} \) within the set \( \mathcal{N}_q^T \) is given by the equation \( RN(\bar{w}, \mathbf{f}) = \sum_{f_1|n_1} \sum_{f_2|n_2} \cdots \sum_{f_d|n_d} RL(\bar{w}, \mathbf{f}) \).

**Computational Tools.** The theoretical tools above show how to transform the size of the sets \( T(\bar{w}, \mathbf{f}) \) to the rank of \( \bar{w} \) among necklaces, and by extension Lyndon words and atranslational necklaces. This leaves the problem of computing the size of \( T(\bar{w}, \mathbf{f}) \). The size of \( T(\bar{w}, \mathbf{f}) \) is computed by partitioning \( T(\bar{w}, \mathbf{f}) \) into \( f_d \) subsets, denoted \( \mathbf{B}(\bar{w}, g_d, j, \mathbf{f}) \) where \( \mathbf{B}(\bar{w}, g_d, j, \mathbf{f}) \) contains every word \( \bar{v} \in \mathcal{L}_Q^T \) where:

- The smallest translation \( t \in \mathcal{Z}_T \) such that \( \bar{v} > \langle \bar{v} \rangle_t \) is of the form \( t = (l_1, l_2, \ldots, l_{d-1}, g_d) \).
- \( j \) is the length of the longest shared prefix of both \( \bar{w} \) and \( \langle \bar{v} \rangle_t \), i.e. \( \bar{w}[1,j] = \langle \bar{v} \rangle_t[1,j] \).

The size of \( T(\bar{w}, \mathbf{f}) \) is given by \( \sum_{t \in \mathcal{Z}_T} \sum_{g_d \in [d]} |\mathbf{B}(\bar{w}, g_d, j, \mathbf{f})| \). The size of \( \mathbf{B}(\bar{w}, g_d, j, \mathbf{f}) \) is computed based on two cases determined by the values of \( j \) and \( g_d \). In the case that \( j + g_d < f_d \):

\[ |\mathbf{B}(\bar{w}, g_d, j, \mathbf{f})| = |\beta(\bar{w}, g_d, 0, \mathbf{f})| \cdot (q^{f_1 \cdot f_2 \cdot \cdots f_{d-1}} - |\beta(\bar{w}_{j+1}, 1, 0, \mathbf{f})| - 1) \cdot (\Theta) \cdot \beta(f_1 \cdot f_2 \cdot \cdots f_{d-1} \cdot (f_d - (g_d + j + 1))) \]

And in the case that \( j + g_d \geq f_d \), the size of \( \mathbf{B}(\bar{w}, g_d, j, \mathbf{f}) \) is given by the equation:

\[ |\mathbf{B}(\bar{w}, g_d, j, \mathbf{f})| = |\beta(\bar{w}, f_d - j - 1, 0, \mathbf{f})| + (|\beta(\bar{w}_{j+1}, 1, 0, \mathbf{f})| - |\beta(\bar{w}_{j+1}, 1, 0, \mathbf{f})|) \cdot (\Theta) \]
Where $\beta(\bar{w}, g_d, j, \bar{f})$ is a set containing every word $\bar{u} \in \Sigma^{f_1, f_2, \ldots, f_{d-1}, g_d}$ with the properties that $\bar{w}_{[1,j]} = \bar{u}_{[1,j]}$ and that every suffix of $\bar{u}$ under any translation from $Z_{[f_1, f_2, \ldots, f_{d-1}]} \ni \bar{w}_{[1,i]}$ is strictly greater than $\bar{w}$, i.e. for every $i \in [g_d]$ and $h \in Z_{[f_1, f_2, \ldots, f_{d-1}]}$, $\bar{w}_{[1,i]} < \langle \bar{u}_{[1,i]} \rangle h$. Further the set $\Theta$ contains the set of unique translations of $\bar{w}_{[1,j]}$, i.e. the set $\{ r \in Z_T : \exists s \in Z_T$ where $s < \langle \bar{w} \rangle r = \langle \bar{w} \rangle_s \}$. This leaves the problem of computing the size of $\beta(\bar{w}, g_d, j, \bar{f})$. Observe that when $i = j$ then either the size of $\beta(\bar{w}, g_d, j, \bar{f})$ is 1, corresponding to the empty word in the case that $i = j = 0$, or 0 when $i > 0$ due to the suffix of length $j$ every word of $\beta(\bar{w}, g_d, j, \bar{f})$ in this case being equal to $\bar{w}_{[1,j]}$. Otherwise when $i \neq j$, as every suffix of $\bar{u} \in \beta(\bar{w}, g_d, j, \bar{f})$ must belong to $\beta(\bar{w}, g_d', j', \bar{f})$ for some $g_d' \leq g_d$ and $j' \in [0, j + 1)$. Therefore the size of $\beta(\bar{w}, g_d, j, \bar{f})$ can be computed in a recursive manner. Explicitly, the size of $\beta(\bar{w}, g_d, j, \bar{f})$ equals:

$$|eta(\bar{w}, g_d, j, \bar{f})| = \begin{cases} 
0 & \text{for } g_d = j, j > 0 \\
1 & \text{for } g_d = j = 0 \\
NS(\bar{w}, j, \bar{f}) \cdot |\beta(\bar{w}, g_d - j, 0, \bar{f})| + |\beta(\bar{w}, g_d, j + 1, \bar{f})| & \text{Otherwise.}
\end{cases}$$

Where $NS(\bar{w}, j, \bar{f})$ returns the number of slices greater than $\bar{w}_j$, defined as:

$$NS(\bar{w}, j, \bar{f}) = (TP(\bar{w}_{j+1}) - TR(\bar{w}_{j+1})) + \sum_{i \in \{d-1\}} \sum_{h_i \in f_i} RA(\bar{w}_j, \bar{h}[i]) \cdot |\bar{h}[i]| \cdot H(i, h, \bar{f}, d)$$

**Theorem 5.** The rank of a $d$-dimensional necklace in the set $\mathcal{N}_q^\pi$ can be computed in $O(N^5)$ time, where $N = \prod_{i=1}^{d} n_i$.

The correctness of this algorithm is shown by first establishing the relationships between the classes of $T(\bar{w}, \bar{f})$, $L(\bar{w}, \bar{f})$, and $A(\bar{w}, \bar{f})$, and the rank of $\bar{w}$ within the sets $\mathcal{N}_q^\pi, \mathcal{L}_q^\pi$ and $\mathcal{A}_q^\pi$. The complexity largely comes from the recursive nature of the algorithm. In general, the cost of determining the size of $T(\bar{w}, \bar{f})$ for every $\bar{T} \in \{ \langle x_1, x_2, \ldots, x_d \rangle \in \Sigma^d : \forall i \in [d], n_i \text{ mod } x_i \equiv 0 \}$ each of these sets requires a set of $n_2^d$ values of $B(\bar{w}, g_d, j, \bar{f})$ in turn requiring $n_d$ words of size $(n_1, n_2, \ldots, n_{d-1})$ to be ranked. As this must be repeated for each dimension, the function $NS$ must be called a total of $O(N^3)$ times. The additional factor of $O(N^2)$ is due to the cost of evaluating $NS$, requiring $O(n_1 + n_2 + \ldots + n_d) \approx O(N)$ calls to $H(i, h, \bar{f}, d)$, itself requiring $O(N)$ time to evaluate.

These results are extended to the fixed content case, where every necklace shares the same Parikh vector $\bar{p}$. The same theoretical tools as unconstrained necklaces are used in the fixed content case. The main difference between these settings, accounting for the increased complexity in the fixed content case, comes from the computational tools. Primarily, when computing the size of $B(\bar{w}, g_d, j, \bar{f})$, it is necessary to subdivide the set $B(\bar{w}, g_d, j, \bar{f})$ based on the Parikh vector of the prefixes. This results in an exponential cost in the size of the alphabet from the $O(N^q)$ potential number of prefix Parikh vectors.

**Theorem 6.** The rank of a $d$-dimensional necklace in the set $\mathcal{N}_q^\pi$ can be computed in $O(N^{6+q})$ time, where $N = \prod_{i=1}^{d} n_i$ and $\bar{p}$ is some given Parikh vector of length $q$.

### 3.4 Unranking

Recall that the unranking problem asks for the necklace $\bar{w}$ with rank $i$ within set $\mathcal{N}_q^\pi$. Let $\bar{w} = \langle \bar{w} \rangle$. Our unranking algorithm works by iteratively determining the prefix of $\bar{w}$, starting with the empty word. At the $j^{th}$ step of the unranking process, the prefix of $\langle \bar{w} \rangle$ of length $j$ has been determined, with the goal being to determine the value of $\bar{w}_{j+1}$. The value of $\bar{w}_{j+1}$ is determined by searching the space of $d-1$ dimensional necklaces for the necklace $\bar{u}$ such that $\bar{w}_{j+1} = \bar{u}_j$. The value of $\bar{u}_j$ is determined using the words $\bar{a}, \bar{b} \in \bar{u}$, where $\bar{a}$ is the canonical representation of $\bar{u}$, and $\bar{b}$ is the largest word in $\bar{u}$. Two words $\bar{A}, \bar{B} \in \Sigma^\pi$ are generated where $\bar{A}$ is the smallest necklace with the prefix $\bar{w}_{[1,j]} : \bar{u}_j$ and $\bar{B}$ the largest necklace with the prefix $\bar{w}_{[1,j]} : \bar{b}$. Using the NextNecklace algorithm given in Section 4, it is possible to find each word in $O(N)$ time. Observe that $\bar{w}_{j+1}$ belongs to necklace class $\bar{u}$ if and only if $RN(\bar{A}, \bar{u}) \leq i \leq RN(\bar{B}, \bar{u})$. Using this as a basis, a binary search is performed over the set $\mathcal{N}_q^{m_1, m_2, \ldots, m_{d-1}}$ to determine the necklace class of $\bar{w}_{j+1}$, starting with the necklace with rank $\mathcal{N}_q^{n_1, m_2, \ldots, m_{d-1}}$, and navigating through the set based on the value of $i$ relative to the ranks of $\bar{A}$ and $\bar{B}$ for each necklace. This requires a $d-1$-dimensional necklace to be unranked at each step.

**Theorem 7.** The $i^{th}$ necklace in $\mathcal{N}_q^\pi$ can be generated (unranked) in $O\left(N^{6+d+1} \cdot \log^d(q) \right)$ time.

**Corollary 1.** The $i^{th}$ necklace in $\mathcal{N}_q^\pi$ can be generated (unranked) in $O(N^{q+7}(d+1)) \log^d(q)$ time.
3.5 The k-centre problem

The last operation this paper presents for the set of multidimensional necklaces is that of the k-centre problem. The difficulty is that we need to select equally spaced centres in implicitly represented sets of objects. For our setting, the k-centre problem for a set of necklaces $N^d_q$ (Problem 7) asks for a set $S$ of $k$ necklaces minimising the objective function $\max_{\mathbf{w} \in N^d_q} \left( \min_{\mathbf{u} \in S} \text{dist}(\mathbf{w}, \mathbf{u}) \right)$, where $\text{dist}(\mathbf{w}, \mathbf{u})$ is some distance function. Motivated by the problem of choosing a distinct set of crystals, we use subwords as a notion of similarity for defining the distance function. To this end, we turn to the the overlap coefficient\cite{8,44,49}. Informally, the overlap coefficient measures of the number of common subwords between necklaces, normalised by the total number of subwords in each necklace. We use $\Omega(\tilde{s}, \tilde{v})$ to denote our overlap based distance between two necklaces.

The graph in this setting corresponds to the set of all necklaces of some given length $n$ over an alphabet $\Sigma$ of size $q$. This setting has some unique properties. While the graph can be completely represented, it is of exponential size relative to the description in terms of $n$ and $q$. Despite this, the graph has a highly symmetric structure due to the nature of necklaces. We show that verifying a solution to the k-centre problem for necklaces can not be done in polynomial time relative to $n$ and $q$ unless $P = NP$, indicating that the k-centre problem itself is likely to be at least NP-hard.

**Theorem 8.** Given a set of $k$ necklaces $S \in N^q_d$ and a distance $\ell$, it is NP-hard to determine if there exists some necklace $\tilde{v} \in N^q_d$ such that $\Omega(\tilde{s}, \tilde{v}) > \ell$ for every $\tilde{s} \in S$ for any dimension $d$.

Despite this challenge, we provide two approximation algorithms for solving the k-centre problem on necklaces, both using de-Bruijn sequences as a basis. A de-Bruijn sequences of order $n$ over the alphabet $\Sigma$ is a cyclic word of length $q^n$ containing every word in $\Sigma^n$ exactly once\cite{9}. In 1D our algorithm splits such a sequence into a set of $k$ centres, requiring some overlap between centres to preserve the property that every word in $\Sigma^n$ appears in some centre at least once. The disconnect between our algorithm and the derived theoretical lower bound is due to some words in $\Sigma^n$ appearing more than once in our set of centres. Figure 7 provides a sketch of the process of dividing such a sequence between a set of $k$ centres.

**Sequence:** 000000100001100010100011001010i101101011011011111
**Centre** | **Word**
---|---
1 | 000000100001100010100
2 | 101001110010101101
3 | 110011010111101011
4 | 000000 0101101011011111

Figure 7: Example of how to split the de Bruijn sequence of order 6 between 4 centres. Highlighted parts are the shared subwords between two centres.

**Theorem 9.** The k-centre problem for $N^q_d$ can be approximated in $O(n \cdot k)$ time with an approximation factor of $1 + f(n, k) = \frac{\log_q (k \cdot n)}{n - \log_q (k \cdot n)} \approx \frac{\log_q (k \cdot n)}{2n(n - \log_q (k \cdot n))}$ and $f(n, k) \to 0$ for $n \to \infty$.

Our second algorithm extends this to the multidimensional setting. At a high level, the idea of this algorithm is to construct an approximation of the de Bruijn torus, the multidimensional equivalent of a de Bruijn sequence, splitting this word between centres analogously to how the de Bruijn sequence is partitioned in the 1D setting. This is achieved by taking the alphabet $\Sigma$ and constructing a new alphabet $\Sigma'$ where each symbol in $\Sigma'$ corresponds to a word in $\Sigma^n$ for some size vector $\Gamma$, where we assume $n_i \mod f_i = 0$ and $f_d = 1$. Any de Bruijn sequence of order $t$ on this new alphabet can be converted to a word $\tilde{w}$ of size $(f_1, f_2, \ldots, f_{d-1}, q t')$ where $F = f_1 \cdot f_2 \cdot \ldots \cdot f_{d-1}$, with the property that $\tilde{w}$ contains every word in $\Sigma^F$ as a subword at least once.

This word $\tilde{w}$ is converted into a set of $k$ centres by first partitioning $\tilde{w}$ into a set $s$ of $k'$ of size $n_1, n_2, \ldots, n_{d-1}$ centres of size $(f_1, f_2, \ldots, f_{d-1}, n_d)$ in the same manner as in the 1D case. Once each centre has been generated, a set of $k$ centres can be constructed by partitioning $s$ into $k$ arbitrary disjoint subsets. Each subset is made into a necklace by concatenating the constitute words into a word of the appropriate size.

**Theorem 11.** The k-centre problem for $N^q_d$ can be approximated in $O(N^2 k)$ time within an approximation factor of $1 + \frac{\log_q (k \cdot N)}{N - \log_q (k \cdot N)} \approx \frac{\log_q (k \cdot N)}{2N(N - \log_q (k \cdot N))}$, where $N = \prod_{i=1}^{d} n_i$. 11
4 Counting of Multidimensional Necklaces

This section provides a comprehensive overview of the equations for counting the number of necklaces, Lyndon words, and a translational necklaces. For both necklaces and Lyndon words, explicit counting is done by application of the Pólya enumeration theorem to the group operations defined in Section 2. Equations 1 and 2 are classical formulas for counting the number of 1D necklaces and 1D Lyndon words respectively. A classical proof for the Necklace Equation is provided by Graham, Knuth and Patashnik [24], while Perrin [40] provides a proof of the Lyndon word Equation.

\[ |\mathcal{A}_q^n| = \frac{1}{n} \sum_{d|n} \phi \left( \frac{n}{d} \right) q^d. \]  
\[ |\mathcal{L}_q^n| = \frac{1}{n} \sum_{d|n} \mu \left( \frac{n}{d} \right) q^d. \]  

In Equation 1, \( \phi(n) \) is Euler’s totient function and in Equation 2, \( \mu(n) \) is the Möbius function. Formally, \( \phi(n) \) gives the number of natural numbers smaller than \( n \) which are co-prime to \( n \), and \( \mu(n) \) returns 1 if \( n \) is a square free integer with an even number of factors, -1 if \( n \) is a square free integer with an even number of factors, and 0 if \( n \) has a square factor. These equations form the starting point for counting multidimensional necklaces.

**Theorem 1.** The number of necklaces of size \( \mathbf{n} \) over an alphabet of size \( q \) is given by the equation:

\[ |\mathcal{N}_q^{\mathbf{n}}| = \frac{1}{N} \sum_{g \in \mathbb{Z}_n^\mathbf{d}} q^{c(g)}. \]

Where \( N = \prod_{i=1}^{d} n_i \) and \( \phi(x) \) is Euler’s totient function.

**Proof.** Recall from the preliminaries that multidimensional necklaces of size \( \mathbf{n} \) are equivalence classes of words in \( \Sigma^\mathbf{d} \) under the group \( \mathbb{Z}_n \times \mathbb{Z}_{n_2} \times \ldots \times \mathbb{Z}_{n_d} \) where \( \times \) denotes the direct product and \( \mathbb{Z}_x \) the cyclic group of order \( x \). A straightforward way to compute the number of necklaces of size \( \mathbf{n} \) is by using the Pólya enumeration formula, giving:

\[ |\mathcal{N}_q^{\mathbf{n}}| = \frac{1}{N} \sum_{g \in \mathbb{Z}_n^\mathbf{d}} q^{c(g)}. \]

Where \( g = (g_1, g_2, \ldots, g_d) \) is some group action in \( \mathbb{Z}_n^\mathbf{d} \) and \( c(g) \) returns the number of cycles from the group action \( g \). Since \( \mathbb{Z}_n^\mathbf{d} \) is formed by the direct product of the cyclic groups, for each group action \( g = (g_1, g_2, \ldots, g_d) \), where \( 1 \leq i_j \leq n_j \). Therefore, the number of necklaces, \( |\mathcal{N}_q^{\mathbf{n}}| \), is rewritten as:

\[ |\mathcal{N}_q^{\mathbf{n}}| = \frac{1}{N} \sum_{g_1=1}^{n_1} \sum_{g_2=1}^{n_2} \cdots \sum_{g_d=1}^{n_d} q^{c(g_1, g_2, \ldots, g_d)}. \]

In order to determine the value of \( c(g) \), consider the permutation induced by \( g \). Given some position \( j = (j_1, \ldots, j_d) \), let \( j' \) be the position following \( j \) in the cycle induced by \( g_i \), i.e. \( j' = j + g \). The coordinate of \( j' \) in the \( i \)-th dimension is equal to the coordinate in the \( i \)-th dimension of \( j \) shifted by \( g_i \). Since this is a cyclic operation, this shift is done modulo the length of dimension \( i \), \( n_i \). This gives \( j'_i = (j_i + g_i) \mod n_i \).

Let \( g' \) denote the group action made by applying \( t \) times operation \( g \) to the identity operation \( I = (0, 0, \ldots, 0) \), i.e. \( I + g + g + \ldots + g \). The length of the cycle induced by some cyclic shift \( g \) is the smallest value \( t > 0 \) such that \( j + g^t = j \). In other words, the length of the cycle equals the number of times \( g \) must be applied to itself to become the identity operation. The length of this cycle is therefore the smallest \( t \) such that for every \( i \), \((j_i + t \cdot g_i) \mod n_i \equiv j_i \).

To compute this, note that \( t \) must be divisible by the smallest value \( l_i \) for each dimension such that \((j_i + l_i \cdot g_i) \mod n_i \equiv j_i \). As such, the smallest value \( t \) may have is the least common multiple of every \( l_i \). For any smaller non-zero value, there is some dimension \( i \) for which \((j_i + t \cdot g_i) \mod n_i \neq j_i \). By the properties of modular addition, it is clear that every cycle has the same length. Therefore, the number of cycles of length \( t \) is \( \frac{N}{t} \).

This is rewritten as follows. Observe that the only possible values for \( l_i \) are divisors of \( n_i \). For each divisor \( f_i \) of \( n_i \), there are \( \phi \left( \frac{n_i}{f_i} \right) \) values for which \( f_i = l_i \). As this is independent in each dimension, this is used to derive the following equation for the number of necklaces:
|Nq]| = \frac{1}{N} \sum_{f_1|n_1} \phi \left( \frac{n_1}{f_1} \right) \sum_{f_2|n_2} \phi \left( \frac{n_2}{f_2} \right) \ldots \sum_{f_d|n_d} \phi \left( \frac{n_d}{f_d} \right) q^{\sum_{i=1}^{d} f_i}. 

Using the set of necklaces as a basis, the next goal is to count the number of Lyndon words.

**Theorem 2.** The number of Lyndon words of size π over an alphabet of size q is given by the equation:

\[ |Lq|^\pi = \sum_{f_1|n_1} \mu \left( \frac{n_1}{f_1} \right) \sum_{f_2|n_2} \mu \left( \frac{n_2}{f_2} \right) \ldots \sum_{f_d|n_d} \mu \left( \frac{n_d}{f_d} \right) |Nq|^{f_1,f_2 \ldots f_d}. \]

Where \( \mu(x) \) is the Möbius function.

**Proof.** In order to derive this algorithm, it is useful to first rewrite the number of necklaces in terms of Lyndon words. Consider the set of necklaces in \( Nq|^\pi \) with a period of size \( \bar{t} \). Note that the period of each necklace corresponds to the minimal word under the translation operation for the necklace class corresponding to the period. More explicitly, given a necklace \( \tilde{w} \in Nq|^\pi \) with a period \( \bar{u} \), for \( \bar{a} \bar{t} \) to be the canonical form of \( \tilde{w} \), \( \bar{a} \bar{t} \) must be the canonical form of \( (\bar{u}) \), as otherwise there would be some translation of \( \bar{a} \bar{t} \) that is smaller than \( \bar{a} \bar{t} \). Therefore, the number of necklaces with a period of size \( \bar{t} \) directly corresponds to the number of Lyndon words of size \( \bar{t} \). Further, any necklace with a period in \( Lq|^\bar{t} \) can not also have a period in \( Lq^|\bar{t} \) for any \( \bar{t} \) without contradiction. Therefore the size of the set of necklaces can be rewritten in terms in terms of the number of Lyndon words as:

\[ |Nq|^\pi = \sum_{f_1|n_1} \sum_{f_2|n_2} \ldots \sum_{f_d|n_d} |Lq|^f_1,f_2,\ldots,f_d. \]

This equation is used to to derive an equation to count the number of Lyndon words using the number of necklaces as a basis. The necklace counting formula is used to compute the number of Lyndon words through repeated application of the Möbius inversion formula, giving:

\[ |Lq|^\pi = \sum_{f_1|n_1} \mu \left( \frac{n_1}{f_1} \right) \sum_{f_2|n_2} \mu \left( \frac{n_2}{f_2} \right) \ldots \sum_{f_d|n_d} \mu \left( \frac{n_d}{f_d} \right) |Nq|^{f_1,f_2 \ldots f_d}. \]

\[ \Box \]

### 4.1 Counting Atranslational necklaces

Related to the concept of aperiodic necklaces are atranslational necklaces. Recall that a necklace \( \tilde{w} \) is atranslational if there exists no cyclic shift \( g \in Zq^\pi \) such that \( g \neq (n_1, n_2, \ldots, n_d) \) and \( (\tilde{w})_g = (\tilde{w}) \). Note that while every aperiodical word is aperiodic, not every aperiodical word is atranslational. As this work is the first to formally characterise these objects, this section provides several key results regarding the structure of aperiodical words. The main result of this section is an equation for counting the number of aperiodical words using Lyndon words, and by extension necklaces, as a basis. Before providing our counting algorithms, we formally prove Proposition [**I**] formally characterising translational Lyndon words.

**Proposition [**I**]** Every word \( \tilde{w} \in Lq|^\pi \) is either in \( Nq|^\pi \) or \( \tilde{w} = \bar{a} \bar{p} : (\bar{a} \bar{p})_g : \ldots : (\bar{a} \bar{p})_{p-1} \) where:

- \( g \) is a translation where \( g_d = p \) and there exists no translation \( r \) such that \( (\bar{a} \bar{p})_r \neq \bar{a} \bar{p} \).
- \( \bar{u} \in Lq^{(n_1 \ldots n_d-1)/p} \), \( t = \frac{n_d}{p} \) and is the smallest value greater than 0 such that \( g^t = I \).

**Proof.** Recall that \( \tilde{w} \in Lq|^\pi \) is used to denote that \( \tilde{w} = \bar{w} \) where \( (\bar{w}) \in Lq|^\pi \). For the sake of contradiction let \( \tilde{w} \in Lq|^\pi \) be an aperiodical word that is neither atranslational nor of the form \( \bar{a} \bar{p} : (\bar{a} \bar{p})_g : \ldots : (\bar{a} \bar{p})_{g^{t-1}} \) for \( \bar{u} \in Lq^{(r/p,n_d-1,\ldots,n_1)/p} \). As \( \tilde{w} \) is not atranslational, let \( g \) be the translation such that \( \tilde{w} = (\bar{w})_g \). Further let \( \bar{u} \) be the prefix of \( \bar{w} \) corresponding to the first \( g_d \) slices. If \( \bar{u} \notin Lq^{(r/p,n_d-1,\ldots,n_1)} \) then...
ū has some period which that is also the period of w. Otherwise note that ⟨ū⟩ = w. Therefore as ⟨w⟩g = w, ⟨w⟩g+1,2g⟩(g_1,g_2,...,g_{d−1}) = ūP. More generally, ⟨w⟩(t−1)g+1,tg⟩(g_1,g_2,...,g_{d−1}) = ūP. This allows ū to be written as ūP : ⟨ū⟩(g_1,g_2,...,g_{d−1}) : ... : ⟨ū⟩(g_1,g_2,...,g_{d−1})−1. Note that if t < n/d, then ⟨w⟩g = (ū)(g_1,g_2,...,g_{d−1}) : ⟨ū⟩(g_1,g_2,...,g_{d−1}) : ... : ⟨ū⟩(g_1,g_2,...,g_{d−1})−1, therefore ⟨w⟩g = ū if and only if ū = (ū)(g_1,g_2,...,g_{d−1}). If ū = ūP : ⟨ū⟩(g_1,g_2,...,g_{d−1}) : ... : ⟨ū⟩(g_1,g_2,...,g_{d−1})−1 = ūP. Hence ū would be periodic. Similarly, if t > n/d and t mod n/d ≡ 0 then for w = ⟨w⟩g, ū = (ū)(g_1,g_2,...,g_{d−1}) meaning ū = ūP. Further, if t > n/d and t mod n/d ≡ 0 then ū has a period of size (n_1,n_2,...,n_{d−1},n/d) = (n/d,1,1,...,1). Therefore for ū to be aperiodic and not a translational it must be of the form ū : ⟨ū⟩(g_1,g_2,...,g_{d−1}) : ... : ⟨ū⟩(g_1,g_2,...,g_{d−1})−1 where t = n/d.

Our techniques for counting atranslational necklaces operates by computing the number of translational (non-atranslational) Lyndon words, corresponding to the size of the set L_π \ Aπ. This is achieved by using the recursive structure given in Proposition 1 with atranslational necklaces as a basis. By showing that any translational Lyndon word can be written in this form of some atranslational necklaces under a set of transformations, it becomes natural to formulate the number of Lyndon words as an equation in terms of atranslational necklaces. Theorem 3 invents this formulation to give the number of atranslational necklaces in terms of Lyndon words and atranslational necklaces of strictly smaller size. As Lyndon words of any size and dimensions can be counted, and 1D atranslational necklaces are equivalent to Lyndon words, this equation in terms of Lyndon word and atranslational words with smaller dimension can be evaluated recursively.

**Theorem 3** The number of atranslational words of size π over an alphabet of size q is given by:

|A_π| = |L_π| - ∑_{i∈[d]} ∑_{|n_i|} \left\{ \begin{array}{ll} 0 & \text{if } l = n_i \\
\frac{d−1}{l} \prod_{t=1}^{d−1} (−μ(n_t)) (−μ(n_d)) |A_q^{n_1,n_2,...,n_{d−1},l}| : H(i,l,π,d) & \text{otherwise} \end{array} \right. 1 < l < n_d

**Theorem 3.** The number of atranslational necklaces of size π over an alphabet of size q is given by:

|A_π| = |L_π| - ∑_{i∈[d]} ∑_{|n_i|} \left\{ \begin{array}{ll} 0 & \text{if } l = n_i \\
\frac{d−1}{l} \prod_{t=1}^{d−1} (−μ(n_t)) (−μ(n_d)) |A_q^{n_1,n_2,...,n_{d−1},l}| : H(i,l,π,d) & \text{otherwise} \end{array} \right. 1 < l < n_d

This section is laid out as follows. Lemmas 1 and 2 provide key combinatorial results that are used to build the equation presented in Lemma 3 to count the number of Lyndon words in terms of atranslational necklaces. These lemmas take advantage of Proposition 1 to build the foundational structure of the translational words. Finally Theorem 3 is restated and formally proven.

Following the characterisation of translational Lyndon words given by Proposition 1 the next obvious question is how to count the number of atranslational necklaces. Lemma 4 shows which translational Lyndon words can be represented in the form outlined by Proposition 1 using as the translational period both some member of L_q^{n_1,n_2,...,n_{d−1},c} and some member of L_q^{n_1,n_2,...,n_{d−1},c,d} for some pair of integers c,d ∈ Z. These relationships form the basis of our counting technique used in Lemma 3 to count the number of Lyndon words in terms of atranslational necklaces.

**Lemma 1.** Let π be a vector of size. Given some value f which is a factor of n_d, and value c which is a factor of f, for any word a ∈ L_q^{n_1,n_2,...,n_{d−1},c} such that a′ : ⟨a⟩_g : ... : ⟨a⟩_g−1 ∈ L_q there exists some word b ∈ L_q^{n_1,n_2,...,n_{d−1},f} such that a′ : ⟨a⟩_g : ... : ⟨a⟩_g−1 = b : ⟨b⟩_g : ... : ⟨b⟩_g−1 where r · c ≤ f.

**Proof.** This claim is shown by considering two cases based on the value of r relative to f. The first case is when r = 0. In this case let g′ = g and b = a′−1 : ⟨a⟩_g. Clearly the Lyndon word a′ : ⟨a⟩_g : ... : ⟨a⟩_g−1 is equivalent to b : ⟨b⟩_g : ... : ⟨b⟩_g−1. In the second case r < 0. If c · r is a factor of f, then either the word a′ : ⟨a⟩_g : ... : ⟨a⟩_g/r : ⟨a⟩_g−r−1 ∈ A_q^{n_1,n_2,...,n_{d−1},f} or a′ : ⟨a⟩_g : ... : ⟨a⟩_g−r−1 is periodic, contradicting the initial assumption. If c · r is not a factor of f, then let r’ = r mod r and t = |r|/r. If a′ : ⟨a⟩_g : ... : ⟨a⟩_g−r−1 is not atranslational then a′ : ⟨a⟩_g : ... : ⟨a⟩_g−r−1 must be periodic with a period in dimension d of at least f. Hence a′ : ⟨a⟩_g : ... : ⟨a⟩_g−r−1 ∈ A_q^{n_1,n_2,...,n_{d−1},f}.

The main challenge is to account for d-dimensional translational Lyndon words made of (d−1)-dimensional translational Lyndon words. To this end the set G(l,π) = \{ (x_1,x_2,...,x_{d−1}) ∈ [π] : x_i mod n_i = 0, for all i ∈ [d] \}
and for some dimension \( i \), there exists no value of \( j \in [\frac{m}{2} - 1] \) such that \( x_i \mod n_j = 0 \) is introduced. This set counts the number of possible translations of a \( d \)-dimensional atranslational word of size \((n_1, n_2, \ldots, n_{d-1}, l)\) that may be used to build a \( d \)-dimensional Lyndon word of size \( \overline{n} \). The following Lemma provides an important step in the computation of the number of \( d-1 \)-dimensional atranslational necklaces that can be used to build a \( d \)-dimensional Lyndon word.

**Lemma 2.** Let \( G(l, \overline{n}) = \{(x_1, x_2, \ldots, x_{d-1}) \in [\overline{n}] : x_i^{n_i/l} \mod n_i = 0\} \), and for some dimension \( i \), there exists no value of \( j \in [\frac{m}{2} - 1] \) such that \( x_i \mod n_j = 0 \). Given some translation \( t \in G(l, (n_1, n_2, \ldots, n_{d-1})), (t_1, t_2, \ldots, t_{d-2}) \in G(l, \overline{n}) \) if and only if \( l = 1 \) and \( n_{d-1} = n_d \).

**Proof.** Observe that \( \frac{n_i}{t} \) must be the smallest translation such that \( t_a \cdot \frac{n_i}{t} \mod n_a = 0 \) for every \( a \in [i - 1] \) and hence \( \frac{n_i}{t} \) must be a factor of \( n_{i+1} \). Additionally, if \( n_{i+1} > \frac{n_i}{t} \), then \( \frac{n_i}{t} \) exists as some value smaller than \( n_{i+1} \) such that \( t_a \cdot \frac{n_i}{t} \mod n_a = 0 \). Hence the only possible value of \( n_{i+1} \) is \( \frac{n_i}{t} \) and for \( n_{i+1} \) to be greater than or equal to \( n_i \), \( l \) must be equal to 1 and therefore \( n_{d+1} = n_1 \). Therefore, given some translation \( t \in G(l, (n_1, n_2, \ldots, n_{d-1})), (t_1, t_2, \ldots, t_{d-2}) \in G(l, \overline{n}) \) if and only if \( l = 1 \) and \( n_{d-1} = n_d \). □

**Lemma 2** provides the basis for generalising the set \( G(l, \overline{n}) \) to count the number of ways a \( d-i \)-dimensional atranslational word can be used to form a \( d \)-dimensional Lyndon word. More explicitly, consider the \( i \)-dimensional atranslational word \( \overline{w} \). To use \( \overline{w} \) as the translational base of some \( d \)-dimensional Lyndon word, note that there must be some translation applied to \( \overline{w} \) at every dimension from \( i \) to \( d \). Let \( \overline{u} = (\langle w_i, t_i \rangle : \ldots : \langle w_i, t_i \rangle)^{(n_i)} : (\langle w_i, t_i \rangle)^{(n_i)} : \ldots : (\langle w_i, t_i \rangle)^{(n_i)}_{l} \). For \( \overline{u} \) to be a Lyndon word, \( h \) must not be \( (g_1, g_2, \ldots, g_i, n_d/l) \) as \( (\langle w_i, t_i \rangle : \ldots : \langle w_i, t_i \rangle)^{(n_i)} : (\langle w_i, t_i \rangle)^{(n_i)} : \ldots : (\langle w_i, t_i \rangle)^{(n_i)}_{l} \).

Using this observation, the following two functions are needed to count the number possible ways an \( i \)-dimensional atranslational word can be used to build a \( d \)-dimensional word. Let \( I(i, l, \overline{n}) \) return the number of dimensions \( j \in [i+1, d] \) where there exists some translation \( g \in G(l, (n_1, n_2, \ldots, n_j)) \) such that \((g_1, g_2, \ldots, g_i, n_d/l) \in G(l, \overline{n}) \). The value of \( I(i, l, \overline{n}) \) can be computed using **Lemma 2** as:

\[
I(i, l, (n_1, n_2, \ldots, n_d)) = \begin{cases} 
0 & i = d \
1 + I(i, l, (n_1, n_2, \ldots, n_{d-1})) & n_i = n_d \\
I(i, l, (n_1, n_2, \ldots, n_{d-1})) & n_i \neq n_d 
\end{cases}
\]

The function \( H(i, l, \overline{n}, d) \) is used to return the number of possible sets of translations that can be used to build a \( d \)-dimensional Lyndon word from \( \overline{w} \). Note that each such set requires \( d - i \) translations if \( l = n_i \), or \( d - i + 1 \) translations if \( l < n_i \). If \( i = d \) then the value of \( H(i, l, \overline{n}, d) \) is either 1, if \( l = n_d \), or \( |G(l, \overline{n})| \) otherwise. If \( i < d \), the number of possible translations of dimensions \( d \) equals the size of \( G(l, \overline{n}) \) minus the number of dimensions where the translation in the lower dimension can be cancelled out by some translation in a higher dimension. Note that if any translation in dimension \( i \) can be cancelled out by some translation in dimensions \( j > i \), then following **Lemma 2** every translation can be. Therefore the value of \( H(i, l, \overline{n}, d) \) is given by the equation

\[
H(i, l, \overline{n}, d) = \prod_{j=i}^{d} \left( 1 - \frac{(\#G(l, \overline{n}) - (\#I(i, l, \overline{n}))) \cdot (\#H(i, l, (n_1, n_2, \ldots, n_{d-1}), d-1))}{l} \right)
\]

Using the functions \( H(i, l, \overline{n}, d) \) and \( I(i, l, \overline{n}) \), the number atranslational necklaces of size \( \overline{n} \) are counted in terms of atranslational necklaces of smaller size and Lyndon words of size \( \overline{n} \). **Lemma 3** shows how to express the number of Lyndon words in terms of atranslational necklaces. **Theorem 3** builds on this to show how to count the number of atranslational necklaces using **Lemma 3**.

**Lemma 3.** The number of \( d \)-dimensional Lyndon words of size \( \overline{n} \) over an alphabet of size \( q \) is given in terms of atranslational necklaces as:

\[
\left| L_q^{\overline{n}} \right| = \left| A_q^{\overline{n}} \right| + \sum_{i \in [d]} \sum_{l | n_i} \left( \sum_{d-1}^{l-1} \mu(n_l) \right) \left( -\mu \left( \frac{n_l}{t} \right) \right) \left| A_q^{n_1, n_2, \ldots, n_{d-1}, l} \right| \cdot H(i, l, \overline{n}, d) \quad 1 < l < n_d
\]
Proof. Note that every Lyndon word is either a translational itself, or of the form $\bar{a}': \langle \bar{a}' \rangle_q: \ldots: \langle \bar{a}' \rangle_q^{d-1}$ for some $\bar{a} \in \mathcal{L}^{n_1,n_2,\ldots,n_d-1,l}$. Following Lemma 1 every Lyndon word of the form $\bar{a}': \langle \bar{a}' \rangle_q: \ldots: \langle \bar{a}' \rangle_q^{g-1}$ can be rewritten as $b: \langle b \rangle_q: \ldots: \langle b \rangle_q^{d-1}$ for some $b \in \mathcal{A}_q^{n_1,n_2,\ldots,n_d-1,l}$. Let $\bar{a}$ be than canonical representation of an atranslational necklace of size $(n_1,n_2,\ldots,n_d-1,l)$. For Lyndon words with a $d$-dimensional translational period there are three cases to consider. If $l = n_d$, then $\bar{a} \in \mathcal{A}_q^{n_1,n_2,\ldots,n_d-1,l}$. If $\frac{n_d}{\mu}$ is prime then for every cyclic shift of $X = (x_1,x_2,\ldots,x_{d-1})$ where $x_i \in 1\ldots n_i-1$ such that $x_i^{\mu d/l} \mod n_i \equiv 0$ and for some $i \neq j \in 1\ldots \frac{n_d}{\mu}$, the word $\bar{a} = \langle \bar{a} \rangle_q X: \ldots: \langle \bar{a} \rangle_q^{d-1}$. The number of words of the form $\bar{a} = \langle \bar{a} \rangle_q: \ldots: \langle \bar{a} \rangle_q^{d-1} \in \mathcal{L}_q^{n_1,n_2,\ldots,n_d-1,l}$ is $|\mathcal{G}(l,\bar{n})| \cdot |\mathcal{A}_q^{n_1,n_2,\ldots,n_d-1,l}|$.

In the case that $\frac{n_d}{\mu}$ is not prime, following Lemma 1 there exists some $d'$ such that $b = \langle \bar{a} \rangle_q: \ldots: \langle \bar{a} \rangle_q^{g'}$ where $b$ has size $(n_1,\ldots,n_l)$. If there are at least two distinct prime factors of $\frac{n_d}{\mu}$, then note that $\bar{a} = \langle \bar{a} \rangle_q: \ldots: \langle \bar{a} \rangle_q^{g'}$ is counted for each prime factor. Let $p$ be the number of distinct prime factors. To avoid over counting, every word of size $(n_1,n_2,\ldots,n_d-1,l)$ needs to be subtracted $p-1$ times. To this end, a new function $P(l)$ is introduced to act as a correction factor.

If $p = 2$ then by setting $P(2) = -1$ the over counting is avoided. If $p = 3$, then as these words were counted three times for each prime factor, then subtracted three times $\frac{n_d}{\mu}$ for each $i$ in the set of prime factors, to avoid under counting these words $P(3)$ must return $1$. One special case is when $\frac{n_d}{\mu}$ has a square prime factor, $\mu$. In this case as $\frac{n_d}{\mu}$ has the same number of distinct primes, $P(\frac{n_d}{\mu})$ must return 0. Repeating this argument, $P(s)$ is $-1$ if $s$ has an even number of prime factors, 1 if $s$ has an odd number of prime factors, and 0 otherwise. Note that this corresponds to $-1(\mu(\frac{n_d}{\mu}))$ where $\mu(\frac{n_d}{\mu})$ is the Möbius function. Further, as $P(1) = 1$, both the prime and non-prime cases can be combined into one case.

The same arguments are applied to the lower dimensional case. Note that the number of possible translations in this case is given by $H(i,l,\bar{n},d)$. This gives the number of Lyndon words with a translational period of size $(n_1,n_2,\ldots,n_i-1,l,1,1,\ldots,1)$ as $|\mathcal{A}_q^{n_1,n_2,\ldots,n_i-1,l,1,1,\ldots,1} \cdot H(i,l,\bar{n},d)|$, where $l$ is a factor of $n_i$. In order to account for under counting, the number of possible Lyndon words is multiplied by $\left( \prod_{t=i+1}^{d-1} -\mu(n_t) \right) (-\mu(\frac{n_d}{\mu}))$. Therefore the total number of Lyndon words of size $\bar{n}$ is equal to:

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

\[ \square \]

**Theorem 3** The number of atranslational necklaces of size $\bar{n}$ over an alphabet of size $q$ is given by:

$$|\mathcal{A}_q^{\bar{n}}| = |\mathcal{L}_q^{\bar{n}}| - \sum_{i \in [d] \cap n_i} \left( \prod_{t=i+1}^{d-1} -\mu(n_t) \right) (-\mu(\frac{n_d}{\mu})) |\mathcal{A}_q^{n_1,n_2,\ldots,n_i-1,l}| \cdot H(i,l,\bar{n},d) 1 < l < n_d$$

**Proof.** It follows from Lemma 3 that the number of translational words in $\mathcal{L}_q^{\bar{n}}$ is given by the equation

$$|\mathcal{L}_q^{\bar{n}} \setminus \mathcal{A}_q^{\bar{n}}| = \sum_{i \in [d] \cap n_i} \left( \prod_{t=i+1}^{d-1} -\mu(n_t) \right) (-\mu(\frac{n_d}{\mu})) |\mathcal{A}_q^{n_1,n_2,\ldots,n_i-1,l}| \cdot H(i,l,\bar{n},d) 1 < l < n_d$$

Hence the number of atranslational necklaces is

$$|\mathcal{A}_q^{\bar{n}}| = |\mathcal{L}_q^{\bar{n}}| - \sum_{i \in [d] \cap n_i} \left( \prod_{t=i+1}^{d-1} -\mu(n_t) \right) (-\mu(\frac{n_d}{\mu})) |\mathcal{A}_q^{n_1,n_2,\ldots,n_i-1,l}| \cdot H(i,l,\bar{n},d) 1 < l < n_d$$

\[ \square \]

### 4.2 Counting Fixed Content Multidimensional Necklaces

Following the results for the unconstrained case, the natural question to ask is if there exists similar formulae for the number of fixed content Necklaces, Lyndon words, and atranslational necklaces. Starting
with \( N_{\mathbf{P}} \), using the arguments from Graham, Knuth and Patashnik [21] the number of necklaces can be computed by considering the possible periodic sub-words. It follows from above that to split along the \( i \)th dimension with a period of \( t_i \), \( \mathbf{P}_j \mod t_i \equiv 0 \) for each letter \( j \). For notation, let \( \mathbf{P} = (P_1, P_2, \ldots, P_q) \). Further let \( \left( \frac{\mathbf{P}}{n} \right) \) denote the multinomial \((p_1, p_2, \ldots, p_q)\). For each subword with periods \( t_1 \) to \( t_D \) there are \( \left( \frac{\mathbf{P}^1}{n} \right) \) possible fixed-content periods. Therefore the total number of fixed content necklaces is:

\[
|N_{\mathbf{P}}| = \frac{1}{N} \sum_{t_1 | \gcd(n_1, \mathbf{P})} \phi \left( \frac{n_1}{d_1} \right) \cdots \sum_{t_D | \gcd(n_D, \frac{P}{d_1} \cdots \frac{P}{d_D-1})} \phi \left( \frac{n_D}{d_D} \right) \left( \frac{\mathbf{P}^1}{n} \right)
\]

Where \( \gcd(n, \mathbf{P}) \) is the greatest common denominator of both \( n \) and every value in the vector \( \mathbf{P} \), i.e. \( \gcd(n, P_1, P_2, \ldots, P_q) \). The number of fixed content Lyndon words can be counted though repeated application of the Möbius inversion formula using the previous arguments as:

\[
L_{\mathbf{P}} = \sum_{d_1 | \gcd(n_1, \mathbf{P})} \mu \left( \frac{n_1}{d_1} \right) \cdots \sum_{d_D | \gcd(n_D, \frac{P}{d_1} \cdots \frac{P}{d_D-1})} \mu \left( \frac{n_D}{d_D} \right) |N_{\mathbf{P}}|_{d_1, \ldots, d_D}
\]

Finally the number of a translational fixed content necklaces is derived using the same arguments as in the unconstrained case. More specifically, the number of a translational necklaces of size \( \mathbf{v} \) is given by:

\[
|A_{\mathbf{P}}^{\mathbf{v}}| = |L_{\mathbf{P}}^{\mathbf{v}}| - \sum_{i \in \mathbf{v}} \sum_{j \| n_i} \left\{ 0, \frac{d-1}{l=1} \prod_{i=1}^{d-1} -\mu(n_i) \right\} \left( -\mu \left( \frac{\mathbf{P}}{\mathbf{v}} \right) \right) |A_{\mathbf{P}/(\mathbf{v}, n_d-1, n_i-l, l)}^{n_1, n_2, \ldots, n_i-1, l} \cdot H(i, l, \mathbf{P}, d) \quad 1 < l < n_d
\]

5 Generating Necklaces

The idea presented here is based on generation of lower dimensional necklaces, generalising the 1D techniques to the higher dimensional setting. For the 1D setting, there have been several approaches for the generation of necklaces in constant amortised time, notably those of Cattell, Ruskey, Sawada, Serra, and Miers [6] and of Fredrickson and Maiorana [13].

Before generating the set of necklace, the idea of a multidimensional prenecklace must be established. Informally, a word is a prenecklace if it is the prefix of the canonical representation of at least one necklace. A prenecklace is a word \( \bar{w} \) of size \((n_1, n_2, \ldots, n_d)\) such that there exists some necklace of size \((n_1, n_2, \ldots, n_d-1, n_d+m)\), for some arbitrary \( m \in \mathbb{N} \) represented by a word \( \bar{u} \) such that \( \bar{u} | \bar{w} = \bar{w} \). The set of prenecklaces of size \( \bar{w} \) over an alphabet of size \( q \) is denoted \( \mathcal{P}_q^{\bar{w}} \) and is assumed to be ordered as in Definition [3]. Note that the canonical representation of every necklace \( \bar{w} \) is a prenecklace as \( \langle \bar{w} \rangle : \langle \bar{w} \rangle \) is the canonical representation of the necklace \( \langle \bar{w} \rangle : \langle \bar{w} \rangle \).

Prenecklaces form the basis for the constant amortised time algorithm due to Cattell, Ruskey, Sawada, Serra, and Miers [6]. Before describing our algorithm, we first provide a reminder of the 1D algorithm. Given a word \( \bar{w} \), let \( \text{lyn}(\bar{w}) \) return the longest prefix of \( \bar{w} \) that is the canonical representation of a Lyndon word. For example, given the word \( \bar{w} = aaabaaab \), \( \text{lyn}(\bar{w}) = aaab \). The 1D algorithm uses these Lyndon prefixes as a means to iterate over the set of all prenecklaces, and by extension necklaces.

**Theorem 2.1.** [10] Let \( \bar{w} \in \mathcal{P}_q^{n-1} \) and let \( p = |\text{lyn}(\bar{w})| \). The word \( \bar{w} : b \) is in \( \mathcal{P}_q^n \) if and only if \( \bar{w}_{n-p} \leq b \leq q \). Furthermore,

\[
|\text{lyn}(\bar{w} : b)| = \begin{cases} p & b = \bar{w}_{n-p} \\ n & b > \bar{w}_{n-p} \end{cases}
\]

Theorem 2.1 is used as the basis for a simple branching algorithm to generate the set of prenecklaces. The idea is to start with the prenecklace corresponding to the empty word, and to branch on the set of possible symbols to extend it. This is repeated in a depth first manner, evaluating the lexicographically smallest branch first at each step, until a depth of \( n \) is reached. Figure [3] provides a visual illustration.

A tempting approach would be to make an alphabet of size equal to the number of necklaces with size \((n_1, \ldots, n_{d-1})\) and to generate the 1D necklaces from that. While this approach would generate a
The remainder of this section proves Theorem 4. First, Lemma 4 provides a key characterisation of prenecklaces. Lemma 4 is strengthened by Lemma 5, which provides the key structural results used as the basis for generating prenecklaces. Lemma 4 is used as the foundation for proving the complexity of Theorem 4, showing the number of prenecklaces that need to be generated to move from one necklace to the next. Finally, Theorem 4 is restated and formally proven.

Before presenting our results on prenecklaces, a set of auxiliary functions are introduced. First given some word $\bar{v} \in \Sigma^n$ let translate($\bar{v}$) return the translation in $g \in \mathbb{Z}_n$ such that $g_1 = TR(\bar{v})_1 + 1 \mod TP(\bar{v})_1$, and $g_i$ is either $TR(\bar{v})_i + 1 \mod TP(\bar{v})_1$, if $g_{i-1} = 0$ and $0 \neq TR(\bar{v})_{i-1}$, or $g_i = TR(\bar{v})_i$ if either $g_{i-1} \neq 0$ or $0 = TR(\bar{v})_i$. Informally, this can be thought of as choosing the next translation in the ordering defined by the index function, while accounting for the periodicity of $\bar{v}$. Secondly, given some
Let $\vec{u} \in \mathcal{N}_q^T$ be a black box function that returns the necklace subsequent to $\vec{u}$ in $\mathcal{N}_q^T$. Finally using these functions as a basis let:

$$\text{NextNecklace}(\vec{w}, i) = \begin{cases} \text{translate}(\vec{w}_i) & \text{TR}(\vec{w}_i) < \text{TP}(\vec{w}_i) \\
\text{NextNecklace}(\vec{w}_i) & \text{TR}(\vec{w}_i) \geq \text{TP}(\vec{w}_i) \end{cases}$$

Informally, $\text{NextNecklace}$ can be thought of as returning the next possible value for the $i^{th}$ slice of the word $\vec{w}$, such that $\vec{w}_{[1,i-1]} : \text{NextNecklace}(\vec{w}, i)$ remains a prenecklace.

**Lemma 4.** A word $\vec{w}$ is a prenecklace if and only if $\vec{w}_1 = \langle \vec{w} \rangle$ and $\vec{w}_{[1,i]} > \langle \vec{w}_{[n_d-i,n_d]} \rangle$ for every $i \in [n_d]$ and $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$.

**Proof.** Observe first that if $\vec{w}_1 \neq \langle \vec{w} \rangle$, then $\langle \vec{w} : \text{TR}(\vec{w}_1) < \vec{w} : \vec{u} \rangle$ for any arbitrary suffix $\vec{u}$, thus $\vec{w}$ can not be a prenecklace. Similarly if $\vec{w}_{[1,i]} < \langle \vec{w}_{[n_d-i,n_d]} \rangle$ for some $i \in [n_d]$ and $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$ then for any $t \in \mathbb{N}$ and word $\vec{w} \in \Sigma_{[n_1,n_2,...,n_d-1]}$, $\langle \vec{w}_{[n_d-i,n_d]} : \vec{u} \rangle : \vec{w}_{[1,n_d-i-1]} \rangle < \vec{w} : \vec{u}$. Hence, there exists no word for which $\vec{w}$ is a prenecklace.

In the other direction, let $\vec{u} = \vec{w} : g(n_1,n_2,...,n_d)$ for some $\vec{w}$ where $\vec{w}_1 = \langle \vec{w} \rangle$ and $\vec{w}_{[1,i]} \leq \langle \vec{w}_{[n_d-i,n_d]} \rangle$ for every $i \in [n_d]$ and $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$. Note that $\vec{u} = \langle \vec{u} \rangle$ if and only if $\vec{u} = \langle \vec{u} \rangle g$ for every $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$. If $\vec{w} = q(n_1,n_2,...,n_d)$ then this condition is satisfied. Alternatively, if $\vec{w} > q(n_1,n_2,...,n_d)$, then $\vec{w}_1 < q(n_1,n_2,...,n_d)$. Let $g \in \Sigma_{[n_1,n_2,...,n_d]}$ be a translation of the form $g = (g_1,g_2,...,g_{n_d-1},n_d + 1)$ for some $t \in [n_d]$. Clearly $\vec{u} = (\vec{u} : g)_{[1,i]}$ if $\vec{u} = (\vec{u} : g)_{[1,i]}$. Similarly, let $r \in \Sigma_{[n_1,n_2,...,n_d]}$ be a translation of the form $r = (r_1,r_2,...,r_{n_d-1},t)$ for some $t \in [n_d]$ and let $r = (r_1,r_2,...,r_{n_d-1})$. Either $\vec{w}_{[1,t]} < (\vec{w}_{n_d-t,n_d}^g)_{[1,i]}$, in which case $\vec{u} = (\vec{u} : r)$, or $\vec{w}_{[1,t]} = (\vec{w}_{n_d-t,n_d}^g)_{[1,i]}$. In the second case, as $\vec{w}_{[1,t]} = (\vec{w}_{n_d-t,n_d}^g)_{[1,i]}$ and $\vec{w} < q(n_1,n_2,...,n_d)$, $\vec{w}_{n_d-t,n_d} < q(n_1,n_2,...,n_d)$. Therefore $\vec{u} = (\vec{u} : r)$, and subsequently $\vec{u} = \langle \vec{u} \rangle$. Hence $\vec{w}$ is a prenecklace.

**Lemma 5.** Let $\vec{w} \in \Sigma^T$ be the $j^{th}$ prenecklace in $\mathcal{P}_q^T$ and let $i \in [n_d]$ be the largest index such that $\vec{w}_1 
eq q(n_1,n_2,...,n_d-1)$. Then the $(j+1)^{th}$ prenecklace in $\mathcal{P}_q^T$, $\vec{u}$ has the structure

$$\vec{u} = \langle \vec{w}_{[1,i-1]} : \text{NextNecklace}(\vec{w}, i) \rangle_{[1,i-1]} \mod i$$

and further $\vec{u}$ is the canonical representation of a necklace if and only if $n_d \mod i = 0$.

**Proof.** This proof is structured as follows. First, it is shown that $\vec{w}_{[1,i-1]} : \text{NextNecklace}(\vec{w}, i)$ is a necklace. It is then shown that no smaller prenecklace that $\vec{u}$ can exist. Finally, it is shown that $\vec{u}$ is the canonical representation of a necklace if and only if $n_d \mod i = 0$.

Consider first that as $\vec{w}$ is a prenecklace then every prefix of $\vec{w}$ must be a prenecklace. As such $\vec{w}''_i = \vec{w}_{[1,i]}$ must be a prenecklace. Therefore, there can exist no translation $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$ for which $\vec{w}_{[1,i]} > \langle \vec{w}_{[n_d-j-1,n_d-j]} \rangle$ for any $j \in [i-1]$. Let $\vec{s} = \text{NextNecklace}(\vec{w}, i)_{[1,i-1]} \mod i$. For $\vec{w}'' : \vec{s}$ to be a necklace, there must be no translation $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$, where $\vec{w''} : \vec{s} > \langle \vec{w} : \vec{g} \rangle$.

Consider the case where $\vec{s} = \text{translate}(\vec{w}_i)$. For the sake of contradiction, assume that under the translation $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$, $\vec{w}'' : \vec{s} > \langle \vec{w''} : \vec{g} \rangle$. In this case there must be some suffix of $\vec{w}$ such that $\vec{w}_{[1,i]} = \langle \vec{w}_{[1,i]} \rangle$. However, this leads to a contradiction as $g$ would have to be greater than or equal to $\langle \text{TP}(\vec{w}_{[1,i-1]}), \text{TP}(\vec{w}_{[1,i-1]}), ..., \text{TP}(\vec{w}_{[1,i-1]}), \text{TR}(\vec{w}_{[1,i-1]}), ..., \text{TR}(\vec{w}_{[1,i-1]}, \text{TR}(\vec{w}_{[1,i-1]})) \rangle$. Further, note that for any translation $g \geq \langle \text{TP}(\vec{w}_{[1,i-1]}), \text{TP}(\vec{w}_{[1,i-1]}), ..., \text{TP}(\vec{w}_{[1,i-1]}), \text{TR}(\vec{w}_{[1,i-1]}), ..., \text{TR}(\vec{w}_{[1,i-1]}, \text{TR}(\vec{w}_{[1,i-1]})) \rangle$ such that $\langle \vec{w''} : \vec{g} \rangle \neq \langle \vec{w} : \vec{g} \rangle$. Therefore, translating $s$ by any translation greater than $\langle \text{TP}(\vec{w}_{[1,i-1]}), \text{TP}(\vec{w}_{[1,i-1]}), ..., \text{TP}(\vec{w}_{[1,i-1]}), \text{TR}(\vec{w}_{[1,i-1]}), ..., \text{TR}(\vec{w}_{[1,i-1]}, \text{TR}(\vec{w}_{[1,i-1]})) \rangle$ leads to representing a word that has previously been looked at.

Consider now the case where $\vec{s} = \text{NextNecklace}(\vec{w}_i)$. For the sake of contradiction, assume again that under the translation $g \in \Sigma_{[n_1,n_2,...,n_d-1]}$, $\vec{w''} : \vec{s} > \langle \vec{w''} : \vec{g} \rangle$. Then there must exist some suffix of $\vec{w}$ such that $\vec{w}_{[1,i]} = \langle \vec{w}_{[1,i]} \rangle$ and where $\langle \vec{g} : \vec{g} \rangle = \langle \vec{g} : \vec{g} \rangle$. However as $\vec{g}$ belongs to a larger necklace class than $\vec{w}_i$, $\vec{w}_i < \langle \vec{g} \rangle$ for every translation $t \in \Sigma_{[n_1,n_2,...,n_d-1]}$. Further, as $\vec{w}_{[1,i]}$ is a prenecklace, $\langle \vec{w}_{[1,i]} \rangle > \langle \vec{w}_{[1,i]} \rangle$. Therefore, $\langle \vec{g} : \vec{g} \rangle = \langle \vec{g} : \vec{g} \rangle$, and hence $\vec{w''} : \vec{s}$ must be the canonical representation of a necklace.

Observe that as $\vec{w''} : \vec{s}$ is the canonical representation of a necklace, any word made by repeating $\vec{w''} : \vec{s}$ must also be a necklace, and by extension any prefix there of must be a prenecklace. Therefore
must be a prenecklace. For the sake of contradiction, let \( \tilde{v} \in \Sigma^n \) be the canonical representation of some prenecklace such that \( \tilde{w} < \tilde{v} < \bar{u} \). Following the above arguments, the prefix of \( \tilde{v} \) of length \( i \) must equal the prefix of \( \bar{u} \) of length \( i \), i.e. \( \tilde{v}[1,i] = \bar{u}[1,i] \). Therefore, if \( \tilde{v} < \bar{u} \) there must exist some index \( j \in [i + 1, n_d] \) such that \( \tilde{v}_j < \bar{u}_j \). Starting with the case where \( j = i + 1 \), if \( \tilde{v}_j < \bar{u}_j \), then \( \tilde{v}_j < \bar{v}_i \) leading to a contradiction as the suffix starting at position \( i + 1 \) of \( \bar{v} \) would be smaller than \( \bar{v} \). Similarly, if \( j = i + 2 \) then if \( \tilde{v}_j < \bar{u}_j, \tilde{v}_j < \bar{v}_j \) and by extension \( \tilde{v}[1,n_d-j] < \bar{v}[j,n_d] \) contradicting the assumption that \( \tilde{v} \) is a prenecklace. More generally, for any arbitrary \( j \in [i + 1, n_d] \) if \( \tilde{v}_j < \bar{u}_j \) then \( \tilde{v}_j < \bar{v}_{j-i} \), implying that \( \tilde{v}_j < \bar{v}_j \mod i \) and by extension \( \tilde{v}[1,n_d-j] < \bar{v}[j,n_d] \). Therefore \( \bar{u} \) must be the prenecklace with rank \( j + 1 \).

In order to show that \( \bar{u} \) is the canonical representation of a necklace if and only if \( n_d \mod i \equiv 0 \), it is sufficient to show that the translational period of \( \tilde{w}' : \bar{s} \) in dimension \( i \) is \( d \). For the sake of contradiction, let there exist some translation \( g \in Z_{n_1,n_2,...,n_d-1} \) and translation \( r \in Z_i \) such that \( \tilde{w}' : \bar{s} = (\langle \tilde{w}' : \bar{s} \rangle)_g \). In this case, \( \bar{s} \) must equal \( \langle \bar{w}_i-1 \rangle_g \). However, as \( \bar{s} > \bar{w}_i, \langle \bar{w}_i-r \rangle_g > \bar{w}_i \). Therefore prefix \( \tilde{w}[1,i] \) can not be a prenecklace as the suffix starting at \( r + 1 \) would be smaller than the corresponding prefix, contradicting the assumption that \( \tilde{w} \) is a prenecklace. Therefore the translational period of \( \tilde{w}' : \bar{s} \) must be \( i \), and hence \( \bar{u} \) can be a necklace if and only if \( n_d \mod i \equiv 0 \).

Lemma 5 provides the basic tool to determine the next prenecklace from a given prenecklace. From a theoretical stand point, this is all that is needed to describe an algorithm in order to generate the next necklace. Formally, by repeatedly applying Lemma 5 to some necklace, the next necklace in the ordering is generated. Lemma 6 formalises the number of times this process needs to be repeated in order to generate the next necklace.

**Lemma 6.** Given \( \bar{w}, \bar{u} \in N^n_i \) such that \( \text{rank}(\bar{u}) = \text{rank}(\bar{w}) + 1 \), let \( \text{Pre}(\bar{w}, \bar{u}) = \{ \bar{v} \in \Sigma^n : \bar{u} > \bar{v} > \bar{w}, \bar{v} \) is a prenecklace \}. The size of \( \text{Pre}(\bar{w}, \bar{u}) \) is at most \( n_d \).

**Proof.** This statement is proven constructively. Let \( \text{NextPrenecklace}(\bar{u}) \) return the smallest prenecklace greater than \( \bar{u} \), using the techniques outlined in Lemmas 5. Let \( \bar{u}^t = \bar{u} \) and let \( \bar{u}^i = \text{NextPrenecklace}(\bar{u}^t-1) \). Similarly let \( \bar{i}^t \in [n_d] \) be the largest index such that \( \bar{u}^t \equiv \bar{q}[n_1,n_2,...,n_{d-1}] \) and let \( \bar{s}^t = \bar{u}^t[i_t] \). Following the arguments given in Lemma 5, every suffix of \( \bar{s}^t \) under any translation \( g \in Z_{n_1,n_2,...,n_d-1} \) where \( g < TP(\bar{s}^t) \) and \( g < TP(\bar{s}^t[i_t]) \) must be strictly greater than \( \bar{s}^t \). Therefore, for any translation \( g \in Z_{n_1,n_2,...,n_d-1,i_t} \), \( \bar{s}^t[1,i_t] \) and hence \( \bar{s}^t \) is the canonical representation of the necklace \( \langle \bar{s}^t \rangle \). Following the construction given in Lemma 5, if \( n_d \mod i_t \equiv 0 \), then \( \bar{u}^t = \langle \bar{u}^t \rangle \). Therefore the number of prenecklaces between \( \bar{w} \) and \( \bar{u} \) equates to the largest value of \( t \) to guarantee that every \( n_d \mod i_t \equiv 0 \). To end observe that following the construction in 5, \( \bar{u}^t_{i_t-1} = \bar{u}^t_{i_t-1} = \bar{u}^t_{i_t-1} \) and further \( \bar{u}^t_{i_t-1} = \bar{q}[n_1,n_2,...,n_{d-1}] \). Therefore \( i_t > i_{t-1} \). Hence the size of \( \text{Pre}(\bar{w}, \bar{u}) \) is at most \( n_d \).

Lemma 6 is used as the basis for determining the complexity of our generation algorithm. At a high level, the \( O(N) \) bound is due to the number of times \( \text{NextPrenecklace} \) needs to be recursively called. Following 6, to transform \( \bar{w} \) representing necklace \( \bar{w} \) to \( \bar{u} \) representing \( \bar{u} \), \( \text{NextPrenecklace} \) needs to be called at most \( n_d \) times. However, for each of these calls, it may be necessary to generate a \( d - 1 \) dimensional necklace, requiring \( n_d-1 \) calls to \( \text{NextPrenecklace} \). Repeating this logic shows that \( \text{NextPrenecklace} \) can be called no more than \( n_1 \cdot n_2 \cdot \ldots \cdot n_d \) times. Theorem 4 formalises this argument.

**Theorem 4.** Let \( \bar{w} \) be a word of size \( \bar{n} \). \( \text{NextNecklace}(\bar{w}) \) returns the smallest word \( \bar{u} > \bar{w} \) such that \( \bar{u} = \langle \bar{u} \rangle \) in \( O(N) \) time.

**Proof.** Following Lemma 6 note that by applying the function \( \text{NextPrenecklace} \) at most \( n_d \) times, the smallest necklace greater than \( \bar{w} \) can be determined. As each call to \( \text{NextPrenecklace} \) requires \( \text{NextNecklace} \) as a subroutine, to determine the next prenecklace of dimensions \( d - 1 \), \( n_d-1 \) prenecklaces of dimensions \( d - 2 \) must be determined. Following this logic, to determine the next prenecklace of dimensions \( d \) at most \( N \) \( \frac{n_d}{n_d-1} \) \( \frac{n_d-1}{n_d-2} \) ... \( \frac{n_1}{n_1-1} \) prenecklaces of dimensions \( i \) must be considered. Therefore a total of \( O(N) \) time is needed to compute all \( n_d \) prenecklaces. As it takes at most \( O(N) \) time to determine if a word is a necklace, this process takes at most \( O(N) \) time.

6 Ranking Multidimensional Necklaces

Informally, the ranking problem, also known as the indexing problem, asks for the number of members of some given ordered set smaller than some element. Unranking is the reverse process, asking for the
words by Kociumaka, Radoszewski, and Rytter [34] who provided an algorithm for converting the size of the set of words belonging to necklace classes smaller than $\bar{w}$ into $\tilde{w}$, the necklace following $\bar{w}$ in the ordering. In the first iteration $\tilde{w}$ is maximal, therefore the slice $\tilde{w}_d$ is incremented, producing the prenecklace $w'$. As $w'$ is not the canonical representation of a necklace, NextPrenecklace must be applied again. In the second iteration the slice $w'_0$ is incremented, giving $\tilde{w}''$ which is the canonical representation of the necklace $\tilde{w}''$, terminating the algorithm.

Within the setting of multidimensional necklaces $N_q$, the rank of a necklace $\tilde{w}$ is the number of necklaces smaller than $\tilde{w}$ under the ordering given in Definition 3. More broadly, we can take any word $\bar{v}$ and determine the number of necklaces with a canonical representation smaller than $\bar{v}$ using the same ordering. In this case, the smallest necklace greater than or equal to $\bar{v}$ is determined using the NextNecklace algorithm given in Theorem 4.

**Theorem 5.** The rank of a $d$-dimensional necklace in the set $N_q$ can be computed in $O(N^5)$ time, where $N = \prod_{i=1}^{d} n_i$.

**Algorithm Outline** Our ranking algorithm uses similar mechanisms to the work of Kociumaka, Radoszewski, and Rytter [34]. At a high level, our ranking technique for is based on transforming the number of words belonging to a necklace class smaller than $\bar{w}$ into the rank of $\bar{w}$ via the ranking algorithm for Lyndon words and anatranslational necklaces. The relationships established in Section 4 are used as a basis for ranking the closely related set of cyclic words known as bracelets [1]. More recently, ranking has been studied for Lyndon words and Necklaces are computed. An overview of the ranking process if given in Figure 11.

This leaves the problem of computing the number of words belonging to a necklace class smaller than $\bar{w}$. A recursive approach similar to the technique presented by Sawada and Williams [54] is used. At a high level, this set of words is partitioned based on two properties; the smallest translation $g \in Z^\pi$ such that $\langle \bar{w}, g \rangle \prec \bar{w}$, and the length $j$ of the longest common prefix between $\langle \bar{w}, g \rangle$ and $\bar{w}$, i.e. the largest value such that $\langle \bar{w}, g \rangle[1..j] = \bar{w}[1..j]$. The size of each of these subsets is computed in a combinatorial manner, by providing a characterisation of words based on the values of $j$ and $g$. In each case, the main computational cost is due to counting the number of words of some length determined by $j$ and $g$ such that each suffix of these words under no translation is strictly greater than the prefix of $\bar{w}$. The number of such words is computed using a recursive formula, observing that if $\bar{v}$ is a word where every suffix is greater than $\bar{w}$ then $\bar{v}[v[0]..\bar{v}[0]]$ must itself be a word such that every suffix is greater than $\bar{w}$.

Before presenting the further technical details of our algorithm, so notation and definitions must be established. For the remainder of this section, it is assumed that the word being ranked is the canonical representation of a necklace. First, it is necessary to define a method of comparing two words of different sizes. In this section, two words $\bar{w} \in \Sigma^\pi$ and $\bar{u} \in \Sigma^T$ are compared if and only if $n_i \mod f_i \equiv 0$ for every $i \in [d]$. As such, given such a pair of words $\bar{w}$ and $\bar{u}$, where $\bar{w}[i_1,i_2,...,i_d] = \bar{u}[i_1 \mod f_1,i_2 \mod f_2,...,i_d \mod f_d]$. Using this notation, a comparison between word $\bar{w}$ and $\bar{u}$
At a high level, the ranking algorithm for a word \( \bar{w} \) in the set of multidimensional necklaces, along with the associated theoretical tools used. This process starts with the set of words belonging to some necklace class smaller than \( \bar{w} \). The size of this set is used to determine the number of aperiodic words belonging to a necklace class smaller than \( \bar{w} \) (shown in Lemma 7) which in turn is used to determine the number of words belonging to atranslational necklaces smaller than \( \bar{w} \) (Lemma 8). From the number of words belonging to atranslational necklaces smaller than \( \bar{w} \), the rank of \( \bar{w} \) is computed, first in terms of atranslational necklaces (Lemma 9), then Lyndon words (Lemma 10) and finally necklaces (Lemma 11).

\[
\begin{align*}
\{v \in \Sigma^\infty, \langle v \rangle < w\} & \quad RN(w) \\
\{v \in \Sigma^\infty, \langle v \rangle < w, v \text{ is aperiodic }\} & \quad RL(w) \\
\{v \in \Sigma^\infty, \langle v \rangle < w, v \text{ is atranslational }\} & \quad RA(w)
\end{align*}
\]

Figure 11: Outline of our ranking technique for some word \( \bar{w} \) in the set of multidimensional necklaces, along with the associated theoretical tools used. This process starts with the set of words belonging to some necklace class smaller than \( \bar{w} \). The size of this set is used to determine the number of aperiodic words belonging to a necklace class smaller than \( \bar{w} \) (shown in Lemma 7) which in turn is used to determine the number of words belonging to atranslational necklaces smaller than \( \bar{w} \) (Lemma 8). From the number of words belonging to atranslational necklaces smaller than \( \bar{w} \), the rank of \( \bar{w} \) is computed, first in terms of atranslational necklaces (Lemma 9), then Lyndon words (Lemma 10) and finally necklaces (Lemma 11).

and \( \bar{u} \) is given as:

**Definition 8.** Let \( \bar{u} \in \Sigma^\infty \) and \( \bar{v} \in \Sigma^\infty \) where \( n_i \mod f_i \equiv 0 \). \( \bar{u} < \bar{v} \) if and only if \( \bar{u}^\infty < \bar{v} \) following Definition 3. Similarly, \( \bar{u} > \bar{v} \) if and only if \( \bar{u}^\infty > \bar{v} \).

At a high level, the ranking algorithm for a word \( \bar{w} \) works by first determining the number of words of size \( \bar{f} = (f_1, f_2, \ldots, f_d) \) smaller than \( \bar{w} \), denoted \( T(\bar{w}, \bar{f}) \), for every \( f_i \) that is a factor of \( n_i \). This value is transformed, first from \( T(\bar{w}, \bar{f}) \) to the number of aperiodic words smaller than \( \bar{w} \), denoted \( L(\bar{w}, \bar{f}) \), and finally to the number of atranslational words smaller than \( \bar{w} \), \( A(\bar{w}, \bar{f}) \). The set \( A(\bar{w}, \bar{f}) \) is then translated into the rank of \( \bar{w} \) within the set of atranslational necklaces \( A'_g \), denoted \( RA(\bar{w}, \bar{f}) \). This rank is then used to calculate the rank within the set of Lyndon words \( RL(\bar{w}, \bar{f}) \). Finally, this rank is translated to the necklace rank \( RN(\bar{w}, \bar{f}) \). Lemmas 7 and 8 show how to transform the size of the sets \( T(\bar{w}, \bar{f}) \) into the size of \( A(\bar{w}, \bar{f}) \). Lemmas 8, 9 and 10 show how to transform the size of the sets \( A(\bar{w}, \bar{f}) \) into the value \( RN(\bar{w}, \bar{f}) \).

In order to compute the size of \( T(\bar{w}, \bar{f}) \), \( T(\bar{w}, \bar{f}) \) is partitioned into the subsets \( B(\bar{w}, g, j, \bar{f}) \). Here \( B(\bar{w}, g, j, \bar{f}) \) contains the set of words \( \bar{v} \in T(\bar{w}, \bar{f}) \) where: (1) \( g \) is the smallest translation such that \( \langle \bar{v} \rangle_g < \bar{w} \) and \( \bar{v} \) has \( \bar{w} \) as a factor of \( n_i \), (2) \( j \) is the length of the longest shared prefix between \( \langle \bar{v}^\infty \rangle_g \) and \( \bar{w} \), i.e. \( \langle \bar{w} \rangle_g \). The size of each set \( B(\bar{w}, g, j, \bar{f}) \) is computed by considering the structure of the words in \( B(\bar{w}, g, j, \bar{f}) \). This requires the size of two further sets to be computed, the number of non-cyclic words where every suffix is greater than \( \bar{w} \), and the number of words of size \( (f_1, f_2, \ldots, f_{d-1}) \) that are smaller than \( \bar{w} \). The first of these sets is the more technical, requiring a new recursive technique to be built which is provided in Subsection 6.2.1.

The remainder of this section proves Theorem 5. For ease of reading, it has been subdivided as follows. Section 6.1 covers the theoretical tools needed to transform the size of the set \( T(\bar{w}, \bar{f}) \) into the rank of \( \bar{w} \). Section 6.2 provides the main tools used to compute the size of \( T(\bar{w}, \bar{f}) \). Finally Theorem 5 is restated and formally proven.

### 6.1 Theoretical Tools

This section covers the theoretical tools that are used to rank necklaces. At a high level, the goal is to start with the set \( T(\bar{w}, \bar{f}) \) and show how to convert it to the rank of \( \bar{w} \), via the sets \( L(\bar{w}, \bar{f}) \) (Lemma 7) and \( A(\bar{w}, \bar{f}) \) (Lemma 8). From the set \( A(\bar{w}, \bar{f}) \), the rank of \( \bar{w} \) is computed, first in the set of atranslational necklaces \( A'_g \) (Lemma 9), then the set of Lyndon words \( L'_g \) (Lemma 10) and finally within the set of necklaces \( N'_g \) (Lemma 11). This section utilizes many of the relationships between the sets of necklaces, Lyndon words, and atranslational necklaces established in Section 4.

**Lemma 7.** The size of \( L(\bar{w}, \bar{f}) \) can be computed in terms of \( T(\bar{w}, \bar{f}) \) using the equation:
\[ |L(\bar{w}, \mathbf{n})| = \sum_{f_1|n_1} \mu \left( \frac{n_1}{f_1} \right) \sum_{f_2|n_2} \mu \left( \frac{n_2}{f_2} \right) \cdots \sum_{f_d|n_d} \mu \left( \frac{n_d}{f_d} \right) |T(\bar{w}, \mathbf{T})| \]

**Proof.** Observe that every word in \( T(\bar{w}, \mathbf{n}) \) is either aperiodic, in which case it is in \( L(\bar{w}, \mathbf{1}) \), or periodic, in which case the period of \( \bar{w} \) is in \( L(\bar{w}, \mathbf{1}) \) where \( f_1 \) is a factor of \( n_1 \). Following the same arguments as given in Section 5, the size of \( T(\bar{w}, \mathbf{n}) \) is equal to \( \sum_{f_1|n_1} \sum_{f_2|n_2} \cdots \sum_{f_d|n_d} |L(\bar{w}, \mathbf{T})| \). By repeated application of the Möbius inversion formula, the size of \( L(\bar{w}, \mathbf{n}) \) can be computed as:

\[ |L(\bar{w}, \mathbf{n})| = \sum_{f_1|n_1} \mu \left( \frac{n_1}{f_1} \right) \sum_{f_2|n_2} \mu \left( \frac{n_2}{f_2} \right) \cdots \sum_{f_d|n_d} \mu \left( \frac{n_d}{f_d} \right) |T(\bar{w}, \mathbf{T})| \]

\[ \square \]

**Lemma 8.** The size of \( A(\bar{w}, \mathbf{n}) \) equals

\[ |L(\bar{w}, \mathbf{n})| - \sum_{i \in [d]} \sum_{i|n_i} \left\{ \begin{array}{ll} 0 & l = n_i \\ \left( \frac{d-1}{d} \right) \left( -\mu \left( \frac{n_i}{f_i} \right) \right) |A(\bar{w}, n_1, n_2, \ldots, n_{i-1}, l)| : H(i, l, \mathbf{n}, d) & l < n_i \end{array} \right. \]

**Proof.** Following the arguments given in Lemma 3, observe that any Lyndon word in \( L(\bar{w}, \mathbf{n}) \) is either a translational, or of the form \( \bar{w} = \langle \bar{w} \rangle_v \). In the latter case, let \( l = [\bar{a}] \). Note that \( \bar{a} \) must be either in \( A(\bar{w}_1), A(\bar{w}_2), \ldots, A(\bar{w}_d) \), if \( l > 1 \) or \( L(\bar{w}_1) \) if \( l = 1 \). Repeating the same arguments as in Lemma 3 allows the size of \( A(\bar{w}, \mathbf{n}) \) to be written as:

\[ |L(\bar{w}, \mathbf{n})| = \sum_{i \in [d]} \sum_{i|n_i} \left\{ \begin{array}{ll} 0 & l = n_i \\ \left( \frac{d-1}{d} \right) \left( -\mu \left( \frac{n_i}{f_i} \right) \right) |A(\bar{w}, n_1, n_2, \ldots, n_{i-1}, l)| : H(i, l, \mathbf{n}, d) & l < n_i \end{array} \right. \]

\[ \square \]

**Lemma 9.** The rank \( RA(\bar{w}, \mathbf{n}) = \frac{1}{N} |A(\bar{w}, \mathbf{n})| \), where \( N = n_1 \cdot n_2 \cdot \ldots \cdot n_d \).

**Proof.** Observe that any aperiodic word of \( \mathbf{n} \) has exactly \( N \) representations. Therefore the number of aperiodical necklaces smaller than \( \bar{w} \) is \( \frac{1}{N} |A(\bar{w}, \mathbf{n})| \). Hence

\[ RA(\bar{w}, \mathbf{n}) = \frac{1}{N} |A(\bar{w}, \mathbf{n})| \]

\[ \square \]

In order to use the rank \( RA(\bar{w}, \mathbf{n}) \) to determine the rank \( RL(\bar{w}, \mathbf{n}) \), it is necessary to consider the special case where \( \bar{w} \) is a translational, aperiodic word. Let \( \bar{u} \in A_{g_1,g_2,\ldots,g_{i-1}} \) be the translational period of \( \bar{w} \), where \( g \in G \left( \bar{w}, n_1, n_2, \ldots, n_i \right) \) is the smallest translation such that \( \bar{w} = \langle \bar{w} \rangle_g \) and \( i \in [d] \) is the smallest index such that \( g_j = 1 \) for all \( j \in [i+1, d] \). Further, let \( \bar{u}[j] \) be the Lyndon word of size \( \left( g_1, g_2, \ldots, g_{i-1}, \frac{n_i}{g_i}, n_{i+1}, \ldots, n_j \right) \) such that \( \bar{u}[j] \) is the smallest index such that \( g_j = 1 \) for all \( j \in [i+1, d] \). Note that \( \bar{u}[j] \) can be written as \( \bar{u}[j] = \bar{u}[j-1] : (\bar{u}[j-1])_{\bar{u}[j-1], \bar{u}[j]} \), for some \( j \in [i+1, d] \). Note that \( \bar{w} \) and \( \bar{u} \) are equal to the sum of the number of translations in \( G \left( l_j, n_1, n_2, \ldots, n_j \right) \) smaller than \( \bar{r}_j \), multiplied by \( H(i, l, \mathbf{n}) \) for every \( j \in [i, d] \). For simplicity, \( S(g, l, (n_1, n_2, \ldots, n_j)) \) return the number of translations in \( G \left( l, n_1, n_2, \ldots, n_j \right) \) smaller than \( g \). Further, let \( U(\bar{w}) \) return either:

- 0 if \( \bar{w} \) is either aperiodical or periodic.
- \( \frac{1}{d} \sum_{j=i}^{d} \left\{ \begin{array}{ll} S(\bar{r}_j, l, (n_1, n_2, \ldots, n_j)) & j = i \\ S(\bar{r}_j, l, (n_1, n_2, \ldots, n_j)) & otherwise \end{array} \right. \) if \( \bar{w} \) is a Lyndon word with a translational period of \( g \). Let \( S(g, l, (n_1, n_2, \ldots, n_j)) \) return the number of translations in \( G \left( l, n_1, n_2, \ldots, n_j \right) \) smaller than \( g \). Using \( U(\bar{w}) \), the number of Lyndon words can be computed from \( RA(\bar{w}, n_1, n_2, \ldots, n_d) \) as follows.
Lemma 10. The rank

\[ RL(\bar{w}, \bar{m}) = RA(\bar{w}, \bar{m}) + U(\bar{w}) + \sum_{i \in [d]} \sum_{l=0}^{l=n_i} \left( -\mu(n_i) \right) \left( -\mu(\frac{n_i}{l}) \right) RA(\bar{w}[1:d], n_1, n_2, \ldots, n_{d-1}) \cdot H(i, l, \bar{m}, d) \quad 1 < l < n_d \]

\[ l = n_i \]

Proof. Note that every necklace smaller than \( \bar{w} \) is either atranslational, in which case it is counted by \( RA(\bar{w}, \bar{m}) \), or is translational. In the latter case following Lemma 3 for each necklace counted by \( RA(\bar{w}[1:d], n_1, n_2, \ldots, n_{d-1}, l) \), there are \( H(i, l, \bar{m}) \) translational necklace counted by \( RL(\bar{w}, \bar{m}) \). Further, if \( \bar{w} \) is a translational Lyndon word of the form \( \bar{v}: \bar{v}_g: \cdots: \bar{v}_g \) where \( \bar{v} = \bar{w} \) for every \( \bar{v} \in [\bar{v}] \). Following Lemma 3 for each necklace counted by \( RA(\bar{w}[1:d], n_1, n_2, \ldots, n_{d-1}) \) as:

\[ RL(\bar{w}, \bar{m}) = RA(\bar{w}, \bar{m}) + U(\bar{w}) + \sum_{i \in [d]} \sum_{l=0}^{l=n_i} \left( -\mu(n_i) \right) \left( -\mu(\frac{n_i}{l}) \right) RA(\bar{w}[1:d], n_1, n_2, \ldots, n_{d-1}) \cdot H(i, l, \bar{m}, d) \quad 1 < l < n_d \]

\[ l = n_i \]

Lemma 11. The rank \( RN(\bar{w}, \bar{m}) = \sum_{f_1[n_1]} \sum_{f_2[n_2]} \cdots \sum_{f_d[n_d]} RL(\bar{w}, \bar{f}) \).

Proof. Observe that every necklace counted by \( RN(\bar{w}, \bar{m}) \) has a period of \( m_i \) where \( m_i \) is a factor of \( |\bar{w}|_i \) for every \( i \in [1..d] \). As \( RL(\bar{w}, \bar{f}) \) counts the rank among aperiodic necklaces of size \( \bar{f} = (f_1, f_2, \ldots, f_d) \), the rank among necklaces is given by:

\[ RN(\bar{w}, \bar{m}) = \sum_{f_1[n_1]} \sum_{f_2[n_2]} \cdots \sum_{f_d[n_d]} RL(\bar{w}, \bar{f}) \]

\[ \square \]

6.2 Computational Tools

Following the theoretical tools provided in Section 6.1, the remaining problem is to compute the size of \( T(\bar{w}, \bar{f}) \). To this end, \( T(\bar{w}, \bar{f}) \) is partitioned into the sets \( B(\bar{w}, g_d, j, \bar{f}) \) such that \( B(\bar{w}, g_d, j, \bar{f}) \) contains every word \( \bar{v} \in T(\bar{w}, \bar{f}) \) where:

- \( g_d \) is the smallest translation in dimension \( d \) of \( \bar{v} \) such that \( \langle \bar{v} \rangle(\theta_1, \theta_2, \ldots, \theta_{d-1}, g_d) < \bar{w} \) for some translation \( \theta \in Z(f_1, f_2, \ldots, f_{d-1}) \).
- \( j \) is the largest value such that \( \langle \bar{v} \rangle(\theta_1, \theta_2, \ldots, \theta_{d-1}, g_d) \}_{[1,j]} = \bar{w}_{[1,j]} \).

Observe that \( |T(\bar{w}, \bar{f})| = \sum_{g_d \in [n_d]} \sum_{j \in [0..n_d-1]} |B(\bar{w}, g_d, j, \bar{f})| \). To compute the size of \( B(\bar{w}, g_d, j, \bar{f}) \), there are two cases to consider based on the values of \( g_d \) and \( j \). The following propositions formalise the structure of each word \( \bar{v} \in B(\bar{w}, g_d, j, \bar{f}) \).

Proposition 2. Given any word \( \bar{v} \in B(\bar{w}, g_d, j, \bar{f}) \), where \( g_d + j < f_d \), \( \bar{v} = \bar{a} : \bar{w}_{[1:j]} : \bar{b} \theta \bar{c} \), where:

- \( \bar{a} \in \Sigma(f_1, f_2, \ldots, f_d) \) is word such that for every \( i \in [g_d] \) and translation \( r \in Z(f_1, f_2, \ldots, g_d) \), \( \langle \bar{a}_{[i,g_d]} \rangle_r \geq \bar{w} \) and \( \langle \bar{a}_{[i,g_d]} \rangle_{\bar{w}_{[1,g_d+r-j]}} > \bar{w}_{[1,g_d+r-j]} \).
- \( \bar{b} \) is some word of size \( (f_1, f_2, \ldots, f_d-1) \) that is smaller than \( \bar{w}_{j+1} \).
- \( \theta \) is a translation in the set \( \Theta = \{ r \in Z(f_1, f_2, \ldots, f_d-1) : \exists s \in Z(f_1, f_2, \ldots, f_d-1) \) where \( s < r \) and \( \langle \bar{w}_{[1,j]} \rangle_r = \langle \bar{w}_{[1,j]} \rangle_s \} \).
• \( \bar{c} \) is an unrestricted word of size \((f_1, f_2, \ldots, f_{d-1}, f_d - (g_d + j + 1))\).

**Proof.** Note that if there exists some subword \((\bar{v}_{[1,g_d]}) < \bar{w}_{[1,j-i]}\) where \(i \in [g_d-1]\), then there exists some translation \(t\) smaller than \(g_d\) such that \(\bar{v}_t < \bar{w}\), contradicting the original assumption. Therefore, the prefix of \(\bar{v}\) of length \(g_d\), \(\bar{a} = \bar{v}_{[1,g_d]}\), must satisfy the property that \((\bar{a}_{[1,g_d]}) \geq \bar{v}_{[1,g_d-i]}\) for every \(i \in [g_d-1]\). Additionally, for \((\bar{v})_g\) to be the smallest translation such that \(\bar{v}_g < \bar{w}\) while sharing a prefix with \(\bar{w}\) of length \(i\), the value of \(\bar{b}\) must be less than \(\bar{w}_{i+1}\). Similarly, if \((\bar{a}_{[1,g_d]}) : \bar{(v)}_r = \bar{w}_{[1,g_d-i]}\) then \(\bar{(b)}_r \geq \bar{w}_{g_d+i+j+1}\). Observe that for \((\bar{a}_{[1,g_d]}) : \bar{(v)}_r = \bar{w}_{[1,g_d-i]}\) to hold, \(\bar{w}_{[1,g_d]}\) must equal \((\bar{w}_{[2,g_d+j+1]}r)\bar{r}\). Therefore, \(\bar{w}_{i+1} \geq \langle \bar{w}_{[j+g_d-f_a,j]} \rangle\bar{r}\) as otherwise \(\bar{w}\) would not be the canonical representation of a necklace. Therefore as \(\bar{w}_{j+1} < \langle \bar{w}_{[j+g_d-f_a,j]} \rangle\bar{r}\) hence if \(\bar{b} < \bar{w}_{j+1}\) then \(\bar{(b)}_r < \bar{w}_{d+g_d+j+1}\). Further every suffix of \(\bar{a}\) must be strictly greater than the prefix of \(\bar{w}\) of the same length. Finally, the suffix of \(\bar{v}\) is unconstrained. □

**Proposition 3.** *(Given any word \(\bar{v} \in \mathcal{B}(\bar{w}, g_d, j, \bar{f})\) where \(g_d + j > f_d\), \(\bar{v} = \langle \bar{v}_{[j+g_d-f_a,j]} \rangle\bar{b}\) where:

- \(s\) is the longest suffix of \(\bar{w}_{[j+g_d-f_a,j]}\) such that \((\bar{w}_{[j-s,j]})r = \bar{w}_{[1,s]}\) for some translation \(s \in Z_{f_1, f_2, \ldots, f_{d-1}}\).
- \(\bar{a}\) is a \((f_1, f_2, \ldots, f_{d-1}, f_d - (j + 1))\) dimensional word for which there exists no translation \(r \in Z_{f_1, f_2, \ldots, f_{d-1}, g_d}\) such that \(\langle \bar{a} \rangle_r < \bar{w}_{[1,g_d]}\).
- \(\bar{b}\) is some word of size \((f_1, f_2, \ldots, f_{d-1})\) that is smaller than \(\bar{w}_{j+1}\), and further \(\langle \bar{b} \rangle_r \geq \bar{w}_{i+1}\).
- \(\theta\) is a translation in the set \(\Theta = \{r \in Z_{(f_1, f_2, \ldots, f_{d-1})} : \langle \# \rangle s \in Z_{(f_1, f_2, \ldots, f_{d-1})} \text{ where } s < r \text{ and } \langle \bar{w}_{(1,j)} \rangle r = \langle \bar{w}_{[1,j]} \rangle s\} \) where:

Proof.** For \(g\) to be the smallest translation such that \(\langle \bar{v} \rangle_g < \bar{w}\) while \(j\) is the length of the longest prefix such that \((\bar{v})_{[1,j]} = \bar{w}_{[1,j]}, \bar{v}_{[g_d + j - f_a + 1]} < \bar{w}_{i+1}\). Further, to ensure that no translation smaller than \(g_d + j - f_a\) is smaller than \(\bar{w}\), \(\langle \bar{a} \rangle_r < \bar{w}_{[1,g_d]}\). Additionally, the subword \(\bar{v}_{[g_d + j + 2 - f_a, g_d]}\) must satisfy the property that \(\langle \bar{v}_{[1,j]} \rangle_r > \bar{w}_{[1,g_d-i]}\) for every \(i \in [g_d + j + 2 - f_a, g_d]\) and \(r \in Z_{f_1, f_2, \ldots, f_{d-1}}\). Further, if \(\langle \bar{b} \rangle_r = \bar{w}_{i+1}\) then for every \(i \in [g_d + j - f_a - s, g_d]\) and \(r \in Z_{f_1, f_2, \ldots, f_{d-1}}\), \((\bar{v}_{[1,j]} \rangle r > \bar{w}_{[1,g_d+i+j+1]}\).

Using Propositions 2 and 3 as a basis, the problem of computing the size of \(\mathcal{B}(\bar{w}, g_d, j, \bar{f})\) can be split into two cases.

**Case 1:** \(g_d + j < f_d\). Following Proposition 2, every word \(\bar{v} \in \mathcal{B}(\bar{w}, g_d, j, \bar{f})\) can be written as \(\bar{a} : \langle \bar{w}_{[1,j]} \rangle \bar{b}\) where:

- \(\bar{a} \in \Sigma^*(f_1, f_2, \ldots, f_{d-1}, g_d)\) is word such that for every \(i \in [g_d]\) and translation \(r \in Z_{(f_1, f_2, \ldots, f_{d-1})}\), \(\langle \bar{a}_{[i,g_d]} \rangle_r \geq \bar{w}\) and \((\bar{a}_{[i,g_d]}) : \bar{w}_{[1,g_d-i]}\).
- \(\bar{b}\) is some word of size \((f_1, f_2, \ldots, f_{d-1})\) that is smaller than \(\bar{w}_{j+1}\).
- \(\theta\) is a translation in the set \(\Theta = \{r \in Z_{(f_1, f_2, \ldots, f_{d-1})} : \langle \# \rangle s \in Z_{(f_1, f_2, \ldots, f_{d-1})} \text{ where } s < r \text{ and } \langle \bar{w}_{[1,j]} \rangle r = \langle \bar{w}_{[1,j]} \rangle s\} \) where:

The main challenge for computing the size of \(\mathcal{B}(\bar{w}, g_d, j, \bar{f})\) is due to calculating the number of possible values of \(\bar{a}\). To this end a new set \(\beta(\bar{w}, i, j, f_1, f_2, \ldots, f_{d-1})\) is introduced containing every word \(\bar{u}\) where:

- The size of \(\bar{u}\) are \((f_1, f_2, \ldots, f_{d-1}, i)\).
- There exists no translation \(h \in Z_{(f_1, f_2, \ldots, f_{d-1})}\) where \(\langle \bar{v}_{[1,i]} \rangle h \leq \bar{w}_{[1,j]}\).
- The first \(j\) slices of \(\bar{u}\) are equal to the first \(j\) slices of \(\bar{w}\) i.e. \(\bar{u}_{[1,j]} = \bar{w}_{[1,j]}\).

When it is clear from context \(\beta(\bar{w}, i, j, f_1, f_2, \ldots, f_{d-1})\) is denoted \(\beta(\bar{w}, i, j, \bar{f})\). A method to compute the size of \(\beta(\bar{w}, i, j, \bar{f})\) is given in Subsection 6.2.1. Using \(\beta(\bar{w}, i, j, \bar{f})\) as a black box, the number of possible values of \(\bar{a}\) is \(|\beta(\bar{w}, i, j, \bar{f})|\). Similarly, the number of possible values of \(\bar{b}\) is given by \(q_1, f_2, \ldots, f_{d-1} - |\beta(\bar{w}_{j+1}, 1, 0, \bar{f})|-1\). The number of possible values of \(\theta\) is equal to the size of the set \(\Theta = \{r \in Z_{\bar{f}} : \langle \# \rangle s \in Z_{\bar{f}}\}\).
where \( s < r \) and \( (\bar{w})_r = (\bar{w})_s \). Finally, the number of values of \( \bar{c} \) is given by \( \bar{q}^{f_1 f_2 \ldots f_{d-1}} (f_d - (g_d + j + 1)) \). Therefore the size of \( B(\bar{w}, g, j, \bar{f}) \) when \( g_d + j < n_d \) is given by:

\[
|\beta(\bar{w}, g_d, 0, \bar{f})| \cdot (\bar{q}^{f_1 f_2 \ldots f_{d-1}} - |\beta(\bar{w}_{j+1}, 1, 0, \bar{f})|) - 1) \cdot |\Theta| \cdot \bar{q}^{f_1 f_2 \ldots f_{d-1}} (f_d - (g_d + j + 1))
\]

**Case 2:** \( g_d + j > f_d \). In this case every word \( \bar{v} \in B(\bar{w}, g_d, j, \bar{f}) \) can be written as \( (\bar{w}_{j+g_d-f_d}) : b) : \bar{a} : (w_{1,j}+g_d-f_d) : \theta \) where:

- \( \bar{a} \) is a d-dimensional word of size \( (f_1, f_2, \ldots, f_{d-1}, f_d - (j + 1)) \) for which there exists no translation \( r \in Z(f_1, f_2, \ldots, f_{d-1}, g_d) \) such that \( (\bar{a})_r < \bar{w}_1, g_d \).
- \( \bar{b} \) is some word of size \( (f_1, f_2, \ldots, f_{d-1}) \) that is smaller than \( \bar{w}_j \).
- \( \theta \) is a translation in the set \( \Theta = \{ r \in Z(f_1, f_2, \ldots, f_{d-1}) : \bar{b} \bar{v} \in Z(f_1, f_2, \ldots, f_{d-1}) \text{ where } s < r \text{ and } (\bar{w}_{1,j} + g_d - f_d) : \theta \}
\]

The number of possible values of \( \theta \) is equal to the size of the set \( \Theta \) as in Case 1. The number of possible values of \( \bar{b} \) in this case is somewhat more complicated than in Case 1. Let \( t \) be the length of the longest suffix of \( \bar{w}_1, j, g_d - f_d \) such that \( \bar{w}_j, t \) is in \( \bar{w}_1, g_d \).

To avoid \( (\bar{v}, \bar{v}) \), for some \( \bar{v} \in Z(f_1, f_2, \ldots, f_{d-1}, g_d - f_d) \) and \( i \neq j \), being smaller than \( \bar{w}_1, g_d \), \( \bar{b} \) must be greater than or equal to \( \bar{w}_1, g_d \).

Note that the number of words greater than \( \bar{w}_1, t \) is given by \( \bar{b}(\bar{w}_1, t, 0, \bar{f}) \). Therefore the number of possible values of \( \bar{b} \) is \( \bar{q}^{f_1 f_2 \ldots f_{d-1}} (f_d - (g_d + j + 1)) - |\beta(\bar{w}_1, 1, 0, \bar{f})| \).

If \( \bar{b} = \bar{w}_1, t \), the number of possible values of \( \bar{b} \) is given by \( |\beta(\bar{w}, f_d - j - 1, 0, \bar{f})| \). Therefore the total number of words of the form \( (\bar{w}_1, j, g_d - f_d) : \theta \) is:

\[
|\beta(\bar{w}, f_d + t - j, t + 1, \bar{f})| + \left( |\beta(\bar{w}_1, t, 1, 0, \bar{f})| + |\beta(\bar{w}_1, 1, 0, \bar{f})| \right) \cdot |\beta(\bar{w}, f_d - j - 1, 0, \bar{f})| \cdot |\Theta|
\]

**6.2.1 Computing the Number of Prefixes Greater than \( \bar{w} \)**

Following Propositions 2 and 3, in order to compute the size of \( T(\bar{w}) \) require the size of the set \( \beta(\bar{w}, i, j, \bar{f}) \) to be computed. Recall that \( \beta(\bar{w}, i, j, \bar{f}) \) contains every word \( \bar{v} \in \Sigma^{f_1, f_2, \ldots, f_{j+1}} \) where:

- For every translation \( h \in Z_\bar{f} \) and index \( k \in [i] \) \( (\bar{v}_{[i-k,i]} h) \).
- The prefix of \( \bar{v} \) of length \( j \) equals the prefix of \( \bar{w} \) of length \( j \), i.e. \( \bar{v}_{[1,j]} = \bar{w}_{[1,j]} \).

The value of \( \beta(\bar{w}, i, j, \bar{f}) \) is given defined recursively, noting that any suffix \( \bar{a} = \bar{v}_{[i-k, i]} \in \beta(\bar{w}, i, j, \bar{f}) \) must also belong to \( \beta(\bar{w}, i, j, \bar{f}) \) for some \( \bar{v}', \bar{v}'' \in [i] \). Additionally, observe that when \( i = j \) then every \( \beta(\bar{w}, i, j, \bar{f}) \) is 0 if \( i > 0 \), or \( \beta(\bar{w}, i, j, \bar{f}) = 1 \) if \( i = 0 \).

This leaves the problem of partitioning \( \beta(\bar{w}, i, j, \bar{f}) \) into sets based of the \( j \)th slice. The key observation is that given some word \( \bar{v} \in \beta(\bar{w}, i, j, \bar{f}) \) where \( \bar{v}_{[1,j]} = \bar{w}_{[1,j]} \), \( \bar{v} \) also belongs to \( \beta(\bar{w}, i, j+1, \bar{f}) \).

On the other hand, given some word \( \bar{u} \in \beta(\bar{w}, i, j, \bar{f}) \) of length \( \bar{u}_{[1,j]} = \bar{w}_{[1,j]} \), the suffix \( \bar{u}_{[j+1,j]} \) belongs to the set \( \beta(\bar{w}, i, j - 1, \bar{f}) \). The following Lemma strengthens this property by showing that any word \( \bar{u} \in \beta(\bar{w}, i, j + 1, \bar{f}) \).

**Lemma 12.** Given any word \( \bar{u} \in \beta(\bar{w}, i, j, \bar{f}) \) and word \( \bar{v} > \bar{w}_{j+1}, \bar{w}_{[1,j]} : \bar{v} : \bar{u} \in \beta(\bar{w}, i + j + 1, j, \bar{f}) \).

**Proof.** As \( \bar{u} \in \beta(\bar{w}, i, j, \bar{f}) \), any suffix of \( \bar{w}_{[1,j]} : \bar{v} : \bar{u} \) starting at index \( t \geq j + 1 \) must satisfy the condition that \( (\bar{w}_{[1,j]} : \bar{v} : \bar{u})_h \in \bar{w}_{[1,j+1]} \) for every \( h \in Z_\bar{f} \). Similarly, for every \( h \in Z_\bar{f} \), \( (\bar{v} : \bar{u})_h \in \bar{w}_{[1,j]} \) as \( \bar{v} > \bar{w}_{j+1} \geq \bar{w}_j \). Further, for any index \( t \in [1,j] \) as \( \bar{w}_{[1,j]} : \bar{v} : \bar{u} : \bar{h} > \bar{w}_{[1,j+1]} \) for every \( h \in \bar{f} \), hence \( \bar{u} : \bar{v} : \bar{u} : \bar{h} > \bar{w}_{[1,j+1]} \). Therefore \( \bar{w}_{[1,j]} : \bar{u} : \bar{u} : \bar{h} > \bar{w}_{[1,j+1]} \).

Following Lemma 12 it is possible to define the size of \( \beta(\bar{w}, i, j, \bar{f}) \) recursively. Let \( NS(\bar{w}, j, \bar{f}) \) return the number of possible slices of size \( f_1, f_2, \ldots, f_{d-1} \) that are greater than \( \bar{w}_j \). Using \( NS(\bar{w}, j, \bar{f}) \) as a black box, the size of \( \beta(\bar{w}, i, j, \bar{f}) \) can be computed as:

\[
\begin{align*}
|\beta(\bar{w}, i, j, \bar{f})| &= \begin{cases} 
1 & i = j, j > 0 \\
NS(\bar{w}, j, \bar{f}) \cdot |\beta(\bar{w}, i - j - 1, 0, \bar{f})| + |\beta(\bar{w}, i + j + 1, \bar{f})| & Otherwise
\end{cases}
\end{align*}
\]

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This leaves the problem of computing \( N_S(\bar{w}, j, \bar{T}) \). This is done by considering two cases. First are the set of slices that belong to a necklace class greater than \( \bar{w}_{j+1} \). The number of such necklaces can be computed as \(|N_q(T)\) \(- RN(\bar{w}_j, f_1, f_2, \ldots, f_d)\) i.e. the number of necklaces of size \((f_1, f_2, \ldots, f_d)\) minus the necklaces smaller than \(\bar{w}_j\). To account for the number of possible translations of each necklace, it is easiest to use the sets of aperiodic words instead. The number of such words are determined by counting the number of atranslational words of size \((f_1, f_2, \ldots, f_i-1, h_1, 1, \ldots, 1)\) for every \(i \in [d]\) and factor \(h_i\) of \(f_i\). This rank is then multiplied by the number of possible translations, given by \(f_1 \cdot f_2 \cdot \ldots \cdot f_{i-1} \cdot h_i\), and \(H(i, h, (f_1, f_2, \ldots, f_d), d)\) to account for the number of necklaces with a translational period in \(T(\bar{w}, f_1, f_2, \ldots, f_d)\). The second case to consider are translations of \(\bar{w}_j\), greater than \(TR(\bar{w}_{j+1})\). This is given by \(TP(\bar{w}_{j+1}) - TR(\bar{w}_j)\). This allows the number of necklaces greater than \(\bar{w}_j\) along with the number of translations of these necklaces to be counted as:

\[
N_S(\bar{w}, j, \bar{T}) = (TP(\bar{w}_{j+1}) - TR(\bar{w}_j)) + \sum_{i \in [d-1]} \sum_{h_i | f_i} RA(\bar{w}_j, \bar{h}[i]) \cdot |\bar{h}[i]| \cdot H(i, h, \bar{T}, d)
\]

Where \(\bar{h}[i] = (f_1, \ldots, f_{i-1}, h_i, 1, \ldots, 1)\) and \(|\bar{h}[i]| = f_1 \cdot f_2 \cdot \ldots \cdot f_{i-1} \cdot h_i\).

### 6.3 Complexity of ranking multidimensional necklaces

The tools are now in place to show the complexity of our ranking algorithm.

Theorem 5. The rank of a \(d\)-dimensional necklace in the set \(N_q^\Pi\) can be computed in \(O(N^5)\) time, where \(N = \prod_{i=1}^{d} n_i\).

Proof. Lemmas 7, 8, 9, 10 and 11 show that to rank \(RN(\bar{w})\), the first step is to compute the size of \(T(\bar{w}, \bar{T})\). Following Lemma 8 to compute the size of \(A(\bar{w}, \bar{T})\), the set \(A(\bar{w}[1], f_1, f_2, \ldots, f_{d-1}, l)\) must be computed for every factor \(l\) of \(f_d\), alongside the set \(L(\bar{w}, T)\) and \(L(\bar{w}_1, f_1, f_2, \ldots, f_{d-1}, l)\). Note that this requires at most \(\log_2(n_d)\) sets to be computed. The size of the set \(L(\bar{w}, f_1, f_2, \ldots, f_{d-1}, l)\) can be computed by computing the size of \(T(\bar{w}, h_1, h_2, \ldots, h_d)\) where \(h_i\) is a factor of \(f_i\). Therefore for \(L(\bar{w}, f_1, f_2, \ldots, f_{d-1}, l)\), the size of at most \(\log_2(N)\) sets \(T(\bar{w}, h_1, h_2, \ldots, h_d)\) must be computed.

Following the above observations, \(T(\bar{w}, \bar{T})\) can be computed by determining the cardinality of the set \(B(\bar{w}, g, j, n_1, n_2, \ldots, n_{d-1})\) using \(n_j^2\) combinations of \(j\) and \(g\). For each pair \(j\) and \(g\), the size of \(\beta(\bar{w}, i, j, n_1, n_2, \ldots, n_{d-1})\) must be computed for some value of \(i\). This is done in a dynamic programming approach. Starting with \(i = j\), the size of \(|\beta(\bar{w}, i, j, \bar{N})|\) is computed using the previously computed values as a basis. As such, the size of \(|\beta(\bar{w}, i, j, \bar{N})|\) for every pair \(i\) and \(j\) can be computed in \(n^2\) time multiplied by the complexity of computing \(NS(\bar{w}, j, \bar{T})\). To compute \(NS(\bar{w}, j, \bar{T})\), \(d \cdot \frac{n^2 \cdot N}{d} = \log_2 \frac{N}{n_d}\) words of size \(d - 1\) must be ranked.

As there are \(n^2\) values of \(\beta(\bar{w}, i, j, \bar{N})\), and \(\log_2 \frac{N}{n_d}\) words of size \(d - 1\) must be ranked for each of the \(n^2\) values of \(\beta(\bar{w}, i, j, \bar{N})\), to precompute every value of \(\beta(\bar{w}, i, j, \bar{N})\), \(n^2 \cdot \log_2 \frac{N}{n_d}\) time is needed, multiplied by the cost of ranking a \(d - 1\) word. If \(d = 2\), then the rank at this step can be computed in \(O(n^2)\) time using existing algorithms due to Sawada and Williams [13]. Hence the size of \(\beta(\bar{w}, i, j, \bar{N})\) for every value of \(i\) and \(j\) can be computed in the two dimensional case in \(O(n_d \cdot N \cdot \log_2 \frac{N}{n_d})\) time. To get the rank of a two dimensional word, a further \(n^2\) time is needed to compute the size of \(T(\bar{w}, \bar{T})\), with \(\log_2(N)\) sets of \(T(\bar{w}, \bar{T})\) to be computed. Therefore the rank of a two dimensional word can be computed in \(O(n^2 \cdot \log_2(N) \cdot N^2 \cdot \log_2 \frac{N}{n_d})\).

Similarly in the three dimensional case, the set of all values of \(\beta(\bar{w}, i, j, \bar{N})\) can be computed in \(O(n^3 \cdot n^2 \cdot \log_2(N) \cdot \log_2(n_1)) = O(N^2 \cdot n^2 \cdot \log_2(N) \cdot \log_2(n_1))\). Thus the complexity of ranking a three dimensional word is \(O(n^3 \cdot \log_2(N) \cdot N^2 \cdot n^2 \cdot \log_2(N) \cdot \log_2(n_1))\) time. In the more general case, a total of \(n^d \cdot \log_2(N)\) words of dimension \(d - 1\) must be ranked. Using the two and three dimensional cases as a base, the total complexity of ranking a \(d\) dimensional word is \(O\left(\prod_{i=2}^{d} n^i \cdot \log_2(n_1)\right) n^2 \leq O(N^5)\). □

### 6.4 Ranking Fixed Content Necklaces

The same tools used in the unrestricted case are used in the fixed content case. As before, the goal is to count the number of words of size \(\bar{T}\) that belong to a necklace class smaller than the ranked word \(\bar{w}\), with the additional constraint that \(F = f_1 \cdot f_2 \cdot \ldots \cdot f_d\) is a factor of \(P_j\) for every \(P_j \in \bar{T}\). The main complexity is generalising the previous approach comes from the constraint on the content. Let
\(T(\bar{w}, i, j, \bar{f}, t, \bar{Q})\) be the set of words of size \(\bar{f}\) with fixed content \(\bar{Q}\) belonging to a necklace class smaller than \(\bar{w}\). As in the unconstrained case, this set is subdivided based on two values \(g_d\) and \(j\). Formally, the set \(B(\bar{w}, \bar{f}, \bar{Q}) \subseteq T(\bar{w}, i, j, \bar{f}, t, \bar{Q})\) contain every word \(\bar{w} \in T(\bar{w}, \bar{f}, \bar{Q})\) where:

- \(h = (h_1, h_2, \ldots, h_{d-1}, g_d)\) is the smallest translation such that \(\langle \bar{v} \rangle_h < \bar{w}\).
- \(j\) is the largest value such that \((\langle \bar{w} \rangle_h)_{1,j} = \bar{w}_{1,j}\).
- \(P(\bar{w}_{1,j}) + \bar{Q} = \bar{Q}\).

In order to compute the size of \(B(\bar{w}, \bar{f}, \bar{Q})\), a generalisation of \(\beta(\bar{w}, i, j, \bar{f})\) is needed. More precisely, due to the constraint on the content, it is necessary not only to count the number of words for which every suffix is greater than \(\bar{w}\), as in \(\beta(\bar{w}, i, j, \bar{f})\), but instead to count the number of such suffixes of the words in \(B(\bar{w}, \bar{f}, \bar{Q})\) for each prefix of \(\bar{w}\). To this end, let \(\gamma(\bar{w}, i, j, \bar{f}, \bar{Q}, t, l)\) return the number of triples \((\bar{x}, \bar{y}, \bar{z})\) where:

- \(\bar{x}\) is a word of size \((f_1, f_2, \ldots, f_{d-1}, i)\) such that every suffix of \(\bar{x}\) belongs to a necklace class larger than the prefix of \(\bar{w}\) of the same length and \(\bar{x}_{1,j} = \bar{w}_{1,j}\).
- \(\bar{y}\) is a word of size \((f_1, f_2, \ldots, f_{d-1})\) such that \(\bar{y} < \bar{w}\).
- \(\bar{z}\) has size \((f_1, f_2, \ldots, f_{d-1}, l)\).
- \(P(\bar{x} : \bar{y} : \bar{z}) = \bar{Q}\).

As with \(\beta(\bar{w}, i, j, \bar{f})\), the problem of computing \(\gamma(\bar{w}, i, j, \bar{f}, \bar{Q}, t, l)\) is solved recursively. In effect, the problem is solved in three stages. First, the number of possible values of \(\bar{x}\) are computed. Secondly, for each value of \(\bar{x}\), the number of possible values of \(\bar{y}\) are computed. Finally, the number of possible values of \(\bar{z}\) are computed using the remaining symbols.

To compute the number of values of \(\bar{x}\), observe that \(\bar{x}_{j+1, i}\) is counted by either \(\gamma(\bar{w}, i-j-1, 0, \bar{f}, \bar{Q} - \gamma(\bar{x}_{j+1}, t, l), j)\), if \(\bar{x}_{j+1} > \bar{w}_{j+1}\), or by \(\gamma(\bar{w}, i, j+1, \bar{f}, \bar{Q} - \gamma(\bar{w}_{j+1}, t, l), t)\) if \(\bar{x}_{j+1} = \bar{w}_{j+1}\). In order to count the number of possible values of \(\bar{x}\) that are greater than \(\bar{w}_{j+1}\), the same approach as in the unrestricted setting is used. Let \(V(\bar{Q}, \bar{f})\) contain every Parikh vector \(\bar{Q}'\) where \(\bar{Q}'_i \leq \bar{Q}_i\) and \(\sum_{i=1}^{d} \bar{Q}'_i = f_1 \cdot f_2 \cdot \cdots \cdot f_{d-1}\). Further let \(X(\bar{w}_{j+1}, \bar{f}, \bar{Q})\) return the number of values of \(\bar{x}_{j+1}\) with a Parikh vector \(\bar{Q}\) that are greater than \(\bar{w}_{j+1}\). \(X(\bar{w}_{j+1}, \bar{f}, \bar{Q})\) is computed in a similar manner to \(\text{NS}(\bar{s}, \bar{j}, \bar{f})\). Formally:

\[
X(\bar{w}_{j+1}, \bar{f}, \bar{Q}) = \left(\left(TP(\bar{w}_{j+1}) - RP(\bar{w}_{j+1})\right) + \sum_{i \in [d-1]} \sum_{h_i / f_i} RA(\bar{w}_{j+1}, \bar{f}_i, \bar{Q}) \cdot (h_1, f_1 \cdot f_2 \cdot \cdots \cdot f_1)\right)
\]

Therefore the number of possible values of \(\bar{x}_{j+1}\) of size \(\bar{f}\) is given by

\[
\sum_{\bar{Q}' \in V(\bar{Q}, \bar{f})} X(\bar{w}_{j+1}, \bar{f}, \bar{Q}')
\]

Similarly the number of possible values of \(\bar{y}\) is the number of words either belonging to a necklace class smaller than \(\langle \bar{w}_{j+1} \rangle\), or belonging to the same necklace class as \(\langle \bar{w}_{j+1} \rangle\), while having a smaller translation. Note that the number of such words for a given Parikh vector \(\bar{Q}\) is given by \(\langle \bar{Q}' \rangle - X(\bar{w}_{j+1}, \bar{f}, \bar{Q}) - 1\). Finally, the number of possible words of size \((f_1, f_2, \ldots, f_{d-1}, l)\) with the Parikh vector \(\bar{Q}\) is given by \(\langle \bar{Q}' \rangle\). Using these observations \(\gamma(\bar{w}, i, j, \bar{f}, \bar{Q}, t, l)\) can be computed as:

\[
\gamma(\bar{w}, i, j, \bar{f}, \bar{Q}, t, l) = \begin{cases} 
\gamma(\bar{w}, i, j+1, \bar{f}, \bar{Q} - \gamma(\bar{w}_{j+1}, t, l)) + \\
\sum_{\bar{Q}' \in V(\bar{Q}, \bar{f})} X(\bar{w}_{j+1}, \bar{f}, \bar{Q}') \cdot \gamma(\bar{w}, i-j-1, 0, \bar{f}, \bar{Q} - \bar{Q}', t, l) & i > j\\
\sum_{\bar{Q}' \in V(\bar{Q}, \bar{f})} (\langle \bar{Q}' \rangle - X(\bar{w}_{j+1}, \bar{f}, \bar{Q}')) \cdot (\langle \bar{Q}' \rangle) & i = j = 0\\
0 & i = j, i > 0
\end{cases}
\]

Using \(\gamma(\bar{w}, i, j, \bar{f}, \bar{Q}, l)\), the size of \(B(\bar{w}, g_d, j, \bar{f}, \bar{Q})\) can be computed in the same manner as the size of \(B(\bar{w}, g_d, j, \bar{f})\). More precisely, two cases are considered based on the value of \(g_d\) and \(j\).
Case 1: $g_d + j \leq f_d$. In this case every word $\bar{v} \in B(\bar{w}, g_d, j, \bar{r}, \bar{q})$ can be written as $\bar{v} : (\bar{w}[1,j] : \bar{b}) : \bar{c}$ where:

- $\bar{a}$ is a $(f_1, f_2, \ldots, f_{d-1}, g_d)$ dimensional word for which there exists no translation $r \in Z_{(f_1, f_2, \ldots, g_d)}$ such that $((\bar{a})_r)_{[1,g_d-r_d]} < (\bar{w})_{[1,g_d-r_d]}$.
- $\bar{b}$ is some word of size $(f_1, f_2, \ldots, f_{d-1})$ that is smaller than $\bar{w}_j$.
- $\theta$ is some translation in $Z_{(f_1, f_2, \ldots, f_{d-1})}$.
- $\bar{c}$ is an unrestricted word of size $(f_1, f_2, \ldots, f_{d-1} - f_d - (g_d + j + 1))$.

Note that $\gamma(\bar{w}, g_d, 0, (f_1, f_2, \ldots, f_{d-1}), \bar{q}, j, n - g_d - j - 1)$ counts the number of possible values of $\bar{a}, \bar{b}$ and $\bar{c}$. The number of possible values of $\theta$ is equal to the size of the set $\Theta = \{ r \in Z_F : \exists s \in Z_{\bar{r}} \text{ where } s < r \text{ and } \langle \bar{w} \rangle_r = \langle \bar{w} \rangle_s \}$. Therefore the size of $B(\bar{w}, g_d, j, \bar{r}, \bar{q})$ when $g_d + j < f_d$ is given by:

$$\gamma(\bar{w}, g_d, 0, (f_1, f_2, \ldots, f_{d-1}), \bar{q}, j, n - g_d - j - 1) \cdot |\Theta|$$

Case 2: $g_d + j > f_d$. In this case every word $\bar{v} \in B(\bar{w}, g_d, j, \bar{r}, \bar{q})$ can be written as $\bar{v} : (\bar{w}[1,j+g_d-f_d] : \bar{b}) : \bar{a}$ where:

- $\bar{a}$ is a $d$-dimensional word of size $(f_1, f_2, \ldots, f_{d-1}, f_d - (j + 1))$ for which there exists no translation $r \in Z_{(f_1, f_2, \ldots, f_{d-1}, g_d)}$ such that $((\bar{a})_r) < (\bar{w})_{[1,g_d]}$.
- $\bar{b}$ is some word of size $(n_1, n_2, \ldots, n_{d-1})$ that is smaller than $\bar{w}_{j+1}$.
- $\theta$ is a translation in the set $\Theta = \{ r \in Z_{(f_1, f_2, \ldots, f_{d-1})} : \exists s \in Z_{(f_1, f_2, \ldots, f_{d-1})} \text{ where } s < r \text{ and } (\bar{w}[1,j])_r = (\bar{w}[1,j+1])_s \}$. The number of possible values of $\theta$ is equal to the size of the set $\Theta$ as in Case 1. The number of possible values of $\bar{b}$ in this case is somewhat more complicated than in Case 1. Let $t$ be the length of the longest suffix of $\bar{w}_{j+g_d-n_{d-1}}$ such that $\bar{w}_{j+g_d-n_{d-1}} = \bar{w}_t$. To avoid $\langle \bar{v} \rangle_\psi$ for some $\psi \in Z_{(f_1, f_2, \ldots, f_{d-1} - n_{d-1} - g_d)}$, being smaller than $\bar{w}$, $\bar{b}$ must be greater than or equal to $\bar{w}_{t+1}$. Let $\gamma'(\bar{w}, i, j, \bar{r}, \bar{q})$ return only the number of words with Parikh vector $\bar{q}$ that are greater than $\bar{w}$ for any translation of the suffix, defined as:

$$\gamma'(\bar{w}, i, j, \bar{r}, \bar{q}) = \begin{cases} \gamma'(\bar{w}, i, j + 1, \bar{r}, \bar{q} - P(\bar{w}_{j+1})) + \\
\sum_{\bar{q}' \in V(\bar{q}, \bar{r})} X(\bar{w}_{j+1}, \bar{r}, \bar{q}') \cdot \gamma'(\bar{w}, i - j, 0, \bar{r}, \bar{q}') & i > j \\
1 & i = j = 0 \\
0 & \text{otherwise.} \end{cases}$$

Using $\gamma'(\bar{w}, i, j, \bar{r}, \bar{q})$, the number of words greater than $\bar{w}_{t+1}$ is given by

$$\sum_{\bar{q} \in V(\bar{r}, \bar{r})} \gamma'(\bar{w}_{t+1}, 1, 0, \bar{r}, \bar{q}).$$

This gives the number of possible values of $\bar{a}$ and $\bar{b}$ where $\bar{a} > \bar{w}_{t+1}$ as

$$\sum_{\bar{q} \in V(\bar{r}, \bar{r})} (\gamma'(\bar{w}_{t+1}, 1, 0, \bar{r}, \bar{q}) - \gamma'(\bar{w}_{j+1}, 1, 0, \bar{r}, \bar{q})) \cdot \gamma'(\bar{w}, i, f_d - (j + 1), \bar{r}, \bar{q}).$$

Accounting for the case where $\bar{a} = \bar{w}_{t+1}$, the size of $B(\bar{w}, g_d, j, \bar{r}, \bar{q})$ when $g_d + j > f_d$ is given by:

$$|\Theta| \cdot \left( \gamma'(\bar{w}, f_d - j, t + 1, \bar{r}, \bar{q} - P(\bar{w}_{t+1})) + \\
\sum_{\bar{q} \in V(\bar{r}, \bar{r})} (\gamma'(\bar{w}_{t+1}, 1, 0, \bar{r}, \bar{q}) - \gamma'(\bar{w}_{j+1}, 1, 0, \bar{r}, \bar{q})) \cdot \gamma'(\bar{w}, i, f_d - (j + 1), \bar{r}, \bar{q}) \right)$$

**Theorem 6.** The rank of a $d$-dimensional necklace in the set $N_F$ can be computed in $O(N^{d+q})$ time, where $N = \prod_{i=1}^d n_i$ and $\bar{r}$ is some given Parikh vector of length $q$. 

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Proof. Following the same arguments from Theorem \[\text{13}\], the complexity cost of this problem comes from computing \(\gamma(\bar{w}, i, j, \bar{f}, \bar{q}, t, l)\). In order to compute \(\gamma(\bar{w}, i, j, \bar{f}, \bar{q}, t, l)\), a dynamic programming approach is used. Observe that \(\gamma(\bar{w}, i, j, \bar{f}, \bar{q}, t, l)\) can be computed in \(|V(\bar{q})|\) steps if \(X(\bar{w}_{j+1}, \bar{f}, \bar{q})\) and \(\gamma(\bar{w}, i - j - 1, 0, \bar{f}, \bar{q} - \bar{q}', t, l)\) have been computed for every \(\bar{q}' \in V(\bar{q})\). Further, \(\gamma(\bar{w}, i, j, \bar{f}, \bar{q}, t, l)\) can be computed in \(O(1)\) time when \(i = j\) if \(X(\bar{w}_{j}, \bar{f}, \bar{q})\) has been precomputed for every value of \(\bar{w}_{j}, \bar{f}\) and \(\bar{q}\).

In order to compute \(X(\bar{w}_{j}, \bar{f}, \bar{q})\), it is necessary to compute the rank of \(\bar{w}_{j}\) among the set of \(d - 1\) atranslational necklaces, in turn requiring \(\gamma(\bar{w}, i, j, \bar{f}, \bar{q}, t, l)\) to be computed for every \(\bar{f} \in \{(m_1, m_2, \ldots, m_{d-2}) : n_1 \mod m_i \equiv 0\}\). By repeating the same arguments from Theorem \[\text{13}\] the problem of ranking fixed content necklaces can be done in an additional factor of \(O(N^{d+1})\), accounting for the number of possible Parikh vectors \(\bar{q}\), and possible values of \(l\). Therefore, the total complexity is \(O(N^{6+d})\).

\[\boxdot\]

7 Unranking Necklaces

This section covers our technique for unranking necklaces. The key idea behind this technique is to build the canonical representation of the \(i^{th}\) necklace, \(\bar{u}\), by iteratively determining each prefix of \(\bar{u}\) in increasing length. The prefix of length \(j + 1\) is determined from the prefix of length \(j\) through a binary search of the space of necklaces of size \((m_1, \ldots, m_{d-1})\). The binary search process is done using the ranking algorithm as a subroutine. When evaluating the necklace \(\bar{v} \in N_{q_1,a_{1},m_{1},\ldots,m_{d-1}}\), the rank of the smallest word with the prefix \(\bar{u}_{1,j} : (\bar{v})\), and the largest word with the prefix \(\bar{u}_{1,j} : (\bar{v})\) are compared. The binary search proceeds by comparing the ranks of these words with \(i\), until some \(d - 1\) dimensional necklace \(\bar{v} \in N_{q_1,a_{1},m_{1},\ldots,m_{d-1}}\) is found such that \(i\) is between the rank of the smallest and largest \(d\)-dimensional necklaces with \(\bar{u}_{1,j} : (\bar{v})\) as a prefix respectively. Once such a necklace \(\bar{v}\) is found, the same process is repeated on the set of possible translations of \(\bar{v}\) to find the prefix of \(\bar{u}\) of length \(j + 1\). This process is repeated until the prefix of length \(n_d\) is found, corresponding directly to \(\bar{u}\).

The remainder of this section is organised as follows. Lemma \[\text{13}\] provides the key tool for determining the number of necklaces sharing a given prefix alongside the primary technical arguments for the unranking process. Using Lemma \[\text{13}\] as a basis, Theorem \[\text{7}\] is restated and formally proven. Finally, Lemma \[\text{14}\] and Corollary \[\text{1}\] are used to extend the Lemma \[\text{13}\] and Theorem \[\text{7}\] respectively to the fixed content setting.

\textbf{Lemma 13.} The number of necklaces in \(|N_q|\) with a given prefix \(\bar{w}\) can be determined in \(O(N^5)\) time.

Proof. Let \(\bar{w}\) be a word of size \((n_1, n_2, \ldots, n_{d-1}, a)\), where \(a \leq n_d\). To determine the number of necklaces with a prefix \(\bar{w}\), two new words \(\bar{\hat{u}}\) and \(\bar{\hat{v}}\) are defined such that \(\bar{u}\) is the smallest necklace reference with the prefix \(\bar{w}\), and \(\bar{v}\) the greatest. The value of \(\bar{u}\) is determined by first constructing the word \(\bar{w}'\) where \(\bar{w}' = \bar{w}_{i} \mod a\). If \(\bar{u}'\) is the canonical representation of the necklace \(\langle \bar{u}' \rangle\), then \(\bar{u}' = \bar{u}'\). Otherwise using Theorem \[\text{4}\] the value of \(\bar{u}\) is computed from \(\bar{u}'\) in at most \(O(N)\) operations. Let \(Q = q^{(n_1, n_2, \ldots, n_{d-1})}\). The word \(\bar{v}\) is defined as being equal to \(\bar{w} : Q^{a-\bar{w}}\). If \(\bar{v}\) is not the canonical representation of \(\bar{v}\) then there exists no necklace with \(\bar{w}\) as a prefix. Otherwise, the number of necklaces with \(\bar{w}\) as a prefix equals \(RN(\bar{v}) - RN(\bar{u}) + 1\).

Using Lemma \[\text{13}\] a recursive unranking algorithm can be built by iteratively building the prefix of the \(i^{th}\) necklace in \(|N_q|\).

\textbf{Theorem 7.} The \(i^{th}\) necklace in \(N_q\) can be generated (unranked) in \(O\left(N^6(d+1) \cdot \log^d(q)\right)\) time.

Proof. The unranking procedure is done in a similar manner to the 1D case as presented by Sawada and Williams \[\text{54}\]. At a high level, the idea is to iteratively generate the necklace by generating prefixes of increasing length. Let \(\bar{w}\) be the canonical representation of the \(j^{th}\) necklace. Further let \(Q = q^{(n_1, n_2, \ldots, n_{d-1})}\), the word of size \((n_1, n_2, \ldots, n_{d-1})\) where every position is occupied by the symbol \(k\). The first slice of \(\bar{w}\) is determined by a binary search. Let \(\bar{u}\) be the canonical representation of \(j^{th}\) necklace of size \((n_1, n_2, \ldots, n_{d-1})\). Note that if \(\bar{u}\) is the first slice of \(\bar{w}\), then the rank of \(\bar{u}\) must be between the rank of the smallest necklace starting with \(\bar{u}\) and the greatest. These necklaces are determined using the same process as laid out in Lemma \[\text{13}\]. Let \(\bar{a}\) be the smallest such word and \(\bar{b}\) the greatest. Therefore \(\bar{a}\) is the first slice of \(\bar{w}\) if and only if \(RN(\bar{a}) \leq i \leq RN(\bar{b})\). Otherwise, depending on the value of \(i\) relative to \(RN(\bar{a})\) and \(RN(\bar{b})\) the next value of \(\bar{u}\) is checked, with \(\bar{u}\) determined by a binary search. Note that there are at
most \( q^N/n_d \) necklaces of size \((n_1, n_2, \ldots, n_{d-1})\), the binary search requires at most \( \log(q^{N/n_d}) = N/n_d \log k \) necklaces to be checked.

For the \( t \)th slice, where \( t \geq 2 \), the process is slightly more complicated. As in the first case, to determine if the \( \langle w_t \rangle = \tilde{a} \), the smallest and largest such words are determined and ranked. To that end, let \( \tilde{a} \) be the smallest possible word that is the canonical representation of a necklace and has the prefix \( w_{[1:t-1]} : \langle \tilde{u} \rangle_{g} \), and let \( \tilde{b} \) be the greatest. The value of \( \tilde{a} \) is computed in \( O(N) \) time following the techniques outlined in Theorem 3. The word \( \tilde{b} = w_{[1:t-1]} : \langle \tilde{u} \rangle_{g} : Q^{n_{t-1} - q} \) where \( g \) is the largest translation such that \( \tilde{u} \neq \langle \tilde{u} \rangle_{g} \). Using these words, \( \langle w_t \rangle = \tilde{a} \) if and only if \( RN(\tilde{a}) \leq t \leq RN(\tilde{b}) \).

The complexity of this process comes from the recursive nature of the algorithm. In dimension \( d \), \( n_d \) slices need to be computed, each requiring at most \( \frac{N}{n_d} \log(q) \) necklaces to be ranked, the ranking having a complexity of \( N^5 \). Note that while determining the necklace that needs to be ranked has a complexity of \( N^2 \), this is not multiplicative with the complexity of ranking as each step is done independently. To determine each of these necklaces, a necklace of size \((n_1, n_2, \ldots, n_{d-1})\) must be unranked, adding an additional complexity of \( \frac{N}{n_d} \cdot \frac{N^5}{n_d} \cdot \log(q) \). As each dimension requires necklaces of the dimension one lower to be computed, the total complexity is \( O \left( \prod_{1 \leq j \leq i} \frac{N^6 \log(q)}{n_d^j} \right) \). In the worst case, where \( n_1 = N \) and \( n_i = 1 \) for \( i \in [2, d] \), this is simplified to \( O \left( \frac{N^6(d+1)}{d^d} \log^d(q) \right) \).

**Lemma 14.** The number of necklaces in the set \( N_{PF}^T \) sharing a given prefix \( \tilde{a} \) can be computed in \( O(n^{6+q}) \) time.

**Proof.** Note that the ranking process outline in Theorem 3 allows the rank of the canonical representation of any necklace to be computed within the set \( N_{PF}^T \) in \( O(n^{6+q}) \) time. Therefore by comparing the ranks of the smallest and largest necklaces sharing \( \tilde{a} \) as a prefix, the number of necklaces in \( N_{PF}^T \) sharing the prefix can be computed. Following Theorem 4, the smallest and largest necklaces can be found in \( O(N) \) time. As the ranking process requires at most \( O(n^{6+q}) \) time, the total complexity of determining the number of necklaces sharing a given prefix is \( O(n^{6+q}) \).

**Corollary 1.** The \( i \)th necklace in \( N_{PF}^T \) can be generated (unranked) in \( O(N(q+7)(d+1)) \log^d(q) \) time.

**Proof.** Fixed content multidimensional necklaces can be unranked in the same manner as unconstrained necklaces, presented in Theorem 7. As in that theorem, a binary search is used over the alphabet \( \Sigma \) to determine the \( i \)th necklace iteratively. Following Lemma 14, the number of necklaces sharing a given prefix can be computed in \( O(n^{6+q}) \) time. The complexity of this process is given by the same arguments as in Theorem 7 with the additional cost due to the added complexity of ranking fixed content necklaces compared to unconstrained necklaces, being \( O(N^{6+q}) \) and \( O(N^5) \) respectively.

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### 8 The \( k \)-Centre Problem on Necklaces

The final set of problems this paper considers is that of choosing a representative sample from some set of necklaces, both in the 1D and multidimensional cases. Here we focus on the local structures, representing the interactions between ions that are as close as possible. The motivation for this approach comes from the energy functions which we look at which have a rapid decrease in energy as distance increases. For example, the Coulomb potential defined as \( \frac{q_i q_j}{r_{ij}} \) tends rapidly towards 0. As such, finding local structures provides a strong basis for exploring the space of possible solutions.

We use the \( k \)-centre problem as a basis to formalise these notions as a computer science problem. The \( k \)-centre problem is a classical graph problem. The \( k \)-centre problem takes as input a weighted graph \( G = (V, E) \) and integer \( k \), with the goal of finding a set \( S \) of \( k \) vertices from \( V \) minimising \( \max_{v \in V} \min_{u \in S} D(v, u) \) where \( D(v, u) \) returns the distance between vertices \( v \) and \( u \). To use the \( k \)-centre problem as a basis for this setting it is necessary to define a distance between words emphasising local differences. The numerous applications of the problem in various areas of computer science have lead to different definitions of connectivity and distance between the vertices depending on the setting at hand.

The \( k \)-center problem is a classical NP-hard problem, such as a great deal of research has been direct to trying to solve it. In the general case the problem is known to not be in \( \text{APX} \) [22]. When the distance satisfies the triangle inequality the problem becomes significantly easier, admitting a polynomial time (relative to the size of the graph) approximation algorithm with a factor of 2 [20, 26]. Further, it is
known no polynomial time approximation algorithm can achieve a factor better than 2 unless \( P = NP \) \cite{28, 38}. Additionally the \( k \)-centre problem is unlikely to be fixed-parameter tractable (FPT) in a context of the most natural parameter \( k \) \cite{12}.

A different form of the \( k \)-centre problem appears in stringology and it was linked with important applications in computational biology; for example to find the approximate gene clusters for a set of words over the DNA alphabet \cite{38}. This problem is also \( NP \)-hard \cite{13, 37}. Despite the hardness of the problem, there are fixed-parameter algorithms \cite{22, 30} allowing some guarantee of optimality for solving the problem. The Closest String problem aims to find a new string within a distance \( d \) to each input of \( n \) strings and such that \( d \) is minimised. The natural generalisation of \( k \)-Closest String problem is of finding \( k \)-center strings of a given length minimising the distance from every string to closest center \cite{18, 32}. This problem has been mainly studied for the popular Hamming distance. The major application of this distance is in the coding theory, but it also has been extensively used in biological applications aiming to discover a region of similarity or to design both probes and primers \cite{36}.

The \( k \)-centre problem can be defined over various distance functions. In this paper we study it in respect to the overlap distance function which can representing the closeness in relation to the number of common subwords and in its turn the closeness of a potential energy in crystals. However, it is not critical for our algorithmic results; all results could be reformulated using other functions by giving of course slightly different approximation bounds. Also, the application of the overlap coefficient, the inverse of which is used as our distance function, is not new and has been successfully used to describe local similarities for “bag-of-words” machine learning techniques, see \cite{17}.

The remainder of this section is organised as follows. Section 8.1 provides the key definitions for this chapter, including the distance used and some fundamental results for the \( k \)-centre problem in this setting. Section 8.2 provides the first approximation algorithm for solving this problem in the 1D case for unconstrained necklaces, using de Bruijn sequences as a basis.

8.1 The Overlap Distance and the \( k \)-Centre Problem

In this section we formally define the \( k \)-centre problem for necklaces. At a high level, the input to our problem is an alphabet of size \( q \), a vector of size \( n = (n_1, n_2, \ldots, n_d) \) that defines the size of the \( d \)-dimensional words, and a positive integer \( k \). Note that in the 1D case \( n \) may be given as a single scalar value, \( n \). The goal is to choose a set \( S \) of \( k \) necklaces from the set \( \Lambda_q^n \) such that the maximum distance between any necklace \( \tilde{\omega} \in \Lambda_q^n \) and the set \( S \) is minimised. Since there is no standard notion of distance between necklaces, our first task is to define one. To this end, we introduce the overlap distance, which aims to capture similarity between crystalline materials emphasising local differences. At a high level, the overlap distance between two necklaces is the inverse of the overlap coefficient between them, in this case 1 minus the overlap coefficient. This can be seen as a natural distance based “bag-of-words” techniques used in machine learning \cite{17}.

Overlap Distance for Necklaces. Our definition of the overlap distance depends of the well studied overlap coefficient, defined for a pair of set \( A \) and \( B \) as \( \frac{|A \cap B|}{\min(|A|, |B|)} \). For notation let \( \mathcal{C}(A, B) \) return the overlap coefficient between two sets \( A \) and \( B \). Observe that \( \mathcal{C}(A, B) \) returns a rational value between 0 and 1, with 0 indicating no common elements and 1 indicating that either \( A \subseteq B \) or \( B \subseteq A \). In the context of necklaces the overlap coefficient \( \mathcal{C}(\tilde{\omega}, \tilde{\nu}) \) is defined as the overlap coefficient between the multisets of all subwords of \( \tilde{\omega} \) and \( \tilde{\nu} \). For some necklace \( \tilde{\omega} \) of size \( n \), the multiset of subwords of size \( l \) contains all \( \tilde{u} \subseteq_\gamma \tilde{w} \). For each subword \( \tilde{u} \) appearing \( m \) times in \( \tilde{w} \), \( m \) copies of \( \tilde{u} \) are added to the multiset. This gives a total of \( N \) subwords of size \( l \) for any \( l \), where \( N = n_1 \cdot n_2 \cdots n_d \). For example, given the necklace represented by \( aaab \), the multiset of subwords of length \( 2 \) are \( \{aa, aa, ab, ba\} = \{aa \times 2, ab, ba\} \). The multiset of all subwords is the union of the multisets of the subwords for every vector of size, having a total size of \( N^2 \); see Figure 12.

To use the overlap coefficient as a distance between \( \tilde{\omega} \) and \( \tilde{\nu} \), the overlap coefficient is inverted so that a value of 1 means \( \tilde{\omega} \) and \( \tilde{\nu} \) share no common subwords while a value of 0 means \( \tilde{\omega} = \tilde{\nu} \). The overlap distance (see example in Figure 12) between two necklaces \( \tilde{\omega} \) and \( \tilde{\nu} \) is \( \mathcal{D}(\tilde{\omega}, \tilde{\nu}) = 1 - \mathcal{C}(\tilde{\omega}, \tilde{\nu}) \). Proposition 4 shows that this distance is a metric distance.

Proposition 4. The overlap distance for necklaces is a metric distance.

Proof. Let \( \tilde{a}, \tilde{b}, \tilde{c} \in \Lambda_q^n \), for some arbitrary vector \( n \in \mathbb{N}^d \) and \( q \in \mathbb{N} \). In order for the overlap distance to satisfy the metric property, \( \mathcal{D}(\tilde{a}, \tilde{b}) \) must be less than or equal to \( \mathcal{D}(\tilde{a}, \tilde{c}) + \mathcal{D}(\tilde{b}, \tilde{c}) \). Rewriting this
Figure 12: Example of the overlap coefficient calculation for a pair of words $ababab$ and $abbabb$. There are 11 common subwords out of the total number of 36 subwords of length from 1 till 6, so $C(ababab, abbabb) = \frac{11}{36}$ and $D(ababab, abbabb) = \frac{25}{36}$.

| A × 3 | B × 4 | Intersection |
|-------|-------|--------------|
| a x 3 | b x 4 | 5            |
| ab x 3, ba x 3 | a x 2, b x 2, b a x 2 | 4        |
| a b a x 3, b a b x 3 | a b x 2, b a b x 2, b a b x 2 | 2        |
| a b b x 3, b a b x 3 | a b b x 2, b a b x 2, b a b x 2 | 0        |
| a b a x 3, b a b x 3 | a b b x 2, b a b x 2, b a b x 2 | 0        |
| Total | 11    |

Figure 13: Example of the overlap distance $D((\tilde{w}), (\tilde{v}))$ for all binary necklaces of length 4.

The $k$-Centre Problem. The goal of the $k$-Centre problem for necklaces is to select a set of $k$ necklaces of size $\mathbf{n}$ over an alphabet of size $q$ that are “central” within the set of necklaces $N_q^\mathbf{n}$. Formally the goal is to choose a set $\mathbf{S}$ of $k$ necklaces such that the maximum distance between any necklace $\tilde{w} \in N_q^\mathbf{n}$ and the nearest member of $\mathbf{S}$ is minimised. Given a set of necklaces $\mathbf{S} \subset N_q^\mathbf{n}$, we use $D(\mathbf{S}, N_q^\mathbf{n})$ to denote the maximum overlap distance between any necklace in $N_q^\mathbf{n}$ and its closest necklace in $\mathbf{S}$.

Problem 1. $k$-Centre problem for necklaces.

**Input:** A size vector of $d$-dimensions $\mathbf{n} \in \mathbb{Z}^d$, an alphabet $\Sigma$ of size $q$, and an integer $k \in \mathbb{Z}$.

**Question:** What is the set $\mathbf{S} \subseteq N_q^\mathbf{n}$ of size $k$ minimising $D(\mathbf{S}, N_q^\mathbf{n})$?

There are two major challenges we have to overcome in order to solve Problem 1: the exponential size of $N_q^\mathbf{n}$, and the lack of structural, algorithmic, and combinatorial results for multidimensional necklaces. We show that the conceptually simpler problem of verifying whether a set of necklaces is a solution for Problem 1 is NP-hard for any dimension $d$.

Problem 2. The $k$-Centre verification problem for necklaces. Given a set of $k$ necklaces $\mathbf{S} \in N_q^\mathbf{n}$ and a distance $\ell$, does there exist some necklace $\tilde{v} \in N_q^\mathbf{n}$ such that $D(\tilde{s}, \tilde{v}) > \ell$ for every $\tilde{s} \in \mathbf{S}$?

**Input:** A size vector of $d$-dimensions $\mathbf{n} \in \mathbb{Z}^d$, an alphabet $\Sigma$ of size $q$, an integer $k \in \mathbb{Z}$, and rational distance $\ell \in \mathbb{Q}$.

**Question:** Does there exists a set $\mathbf{S} \subseteq N_q^\mathbf{n}$ of size $k$ such that $D(\mathbf{S}, N_q^\mathbf{n}) \leq \ell$?

**Theorem 8.** Given a set of $k$ necklaces $\mathbf{S} \in N_q^\mathbf{n}$ and a distance $\ell$, it is NP-hard to determine if there exists some necklace $\tilde{v} \in N_q^\mathbf{n}$ such that $D(\tilde{s}, \tilde{v}) > \ell$ for every $\tilde{s} \in \mathbf{S}$ for any dimension $d$.

**Proof.** This claim is proven via a reduction from the Hamiltonian cycle problem on bipartite graphs to Problem 1 in 1D. Note that if the problem is hard in the 1D case, then it is also hard in any dimension $d \geq 1$ by using the same reduction for necklaces of size $(n_1, 1, 1, \ldots, 1)$. Let $G = (V, E)$ be a bipartite graph containing an even number $n \geq 6$ of vertices. The alphabet $\Sigma$ is constructed with size $n$ such that there is a one to one correspondence between each vertex in $V$ and symbol in $\Sigma$. Using $\Sigma$ a set $\mathbf{S}$ of necklaces is constructed as follows. For every pair of vertices $u, v \in V$ where $(u, v) \notin E$, the necklace...
corresponding to the word \((uv)^{n/2}\) is added to the set of centres \(S\). Further the word \(v^n\), for every \(v \in V\), is added to the set \(S\).

For the set \(S\), we ask if there exists any necklace in \(\mathcal{N}_{2s}^q\) that is further than a distance of \(1 - \frac{3}{n}\). For the sake of contradiction, assume that there is no Hamiltonian cycle in \(G\), and further that there exists a necklace \(\tilde{w} \in \mathcal{N}_{2s}^q\) such that the distance between \(\tilde{w}\) and every necklace \(\tilde{v} \in S\) is greater than \(1 - \frac{3}{n}\). If \(\tilde{w}\) shares a subword of length 2 with any necklace in \(S\) then \(\tilde{w}\) would be at a distance of no less than \(1 - \frac{2}{n}\) from \(S\). Therefore, as every subword of length 2 in \(S\) corresponds to a edge that is not a member of \(E\), every subword of length 2 in \(\tilde{w}\) must correspond to a valid edge.

As \(\tilde{w}\) cannot correspond to a Hamiltonian cycle, there must be at least one vertex \(v\) for which the corresponding symbol appears at least 2 times in \(\tilde{w}\). As \(G\) is bipartite, if any cycle represented by \(\tilde{w}\) has length greater than 2, there must exist at least one vertex \(u\) such that \((v, u) \notin E\). Therefore, the necklace \((uv)^{n/2}\) is at a distance of no more than \(1 - \frac{2}{n}\) from \(\tilde{w}\). Alternatively, if every cycle represented by \(\tilde{w}\) has length 2, there must be some vertex \(v\) that is represented at least 3 times in \(\tilde{w}\). Hence in this case \(\tilde{w}\) is at a distance of no more than \(1 - \frac{2}{n}\) from the word \(v^n \in S\). Therefore, there exists a necklace at a distance of greater than \(1 - \frac{3}{n}\) if and only if there exists a Hamiltonian cycle in the graph \(G\). Therefore, it is NP-hard to verify if there exists any necklace at a distance greater than \(l\) for some set \(S\).

The combination of this negative result with the exponential size of \(\mathcal{N}_{2s}^q\) relative to \(n\) and \(q\) makes finding an optimal solution for Problem 4 exceedingly unlikely. As such the remainder of our work on the \(k\)-centre problem for necklaces focuses on approximation algorithms. Lemma 15 provides a lower bound on the optimal distance.

**Lemma 15.** Let \(S \subseteq \mathcal{N}_{2s}^q\) be an optimal set of \(k\) centres minimising \(\mathcal{D}(S, \mathcal{N}_{2s}^q)\) then \(\mathcal{D}(S, \mathcal{N}_{2s}^q) \geq 1 - \frac{\log_q(k \cdot N)}{N}\).

**Proof.** We first prove the lemma for the 1D case, then extend the proof to the multidimensional setting.

Recall that the distance between any pair of necklaces \(\tilde{u}\) and \(\tilde{v}\) is determined by the overlap coefficient and by extension the number of shared subwords between \(\tilde{u}\) and \(\tilde{v}\). Hence the distance between the furthest necklace \(\tilde{w} \in \mathcal{N}_{2s}^q\) and the optimal set \(S\) is bound from below by determining an upper bound on the number of shared subwords between \(\tilde{w}\) and the words in \(S\). For the remainder of this proof let \(\tilde{w}\) to be the necklace furthest from the optimal set \(S\). Further for the sake of determining an upper bound, the set \(S\) is treated as a single necklace \(\tilde{S}\) of length \(n \cdot k\). This may be thought of as the necklace corresponding to the concatenation of each necklace in \(S\). Note that the length of \(\tilde{S}\) is \(k \cdot n\). As the distance between \(\tilde{w}\) and \(\tilde{S}\) is no more than the distance between \(\tilde{w}\) and any \(\tilde{v} \in S\), the distance between \(\tilde{w}\) and \(\tilde{S}\) provides a lower bound on the distance between \(\tilde{w}\) and \(S\).

In order to determine the number of subwords shared by \(\tilde{w}\) and \(\tilde{S}\), consider first the subwords of length 1. In order to guarantee that \(\tilde{w}\) shares at least one subword of length 1, \(\tilde{S}\) must contain each symbol in \(\Sigma\), requiring the length of \(\tilde{S}\) to be at least \(q\). Similarly, in order to ensure that \(\tilde{w}\) shares two subwords of length 1 with \(\tilde{S}\), \(\tilde{S}\) must contain 2 copies of every symbol on \(\Sigma\), requiring the length of \(\tilde{S}\) to be at least \(2q\). More generally for \(\tilde{S}\) to share \(i\) subwords of length 1 with \(\tilde{w}\), \(\tilde{S}\) must contain \(i\) copies of each symbol in \(\Sigma\), requiring the length of \(\tilde{S}\) to be at least \(i \cdot q\). Hence the maximum number of subwords of length 1 that \(\tilde{w}\) can share with \(\tilde{S}\) is either \([\frac{n \cdot k}{q}]\), if \([\frac{n \cdot k}{q}] \leq n\), or \(n\) otherwise.

In the case of subwords of length 2, the problem becomes somewhat more complicated. Note that in order to share a single word of length 2, it is not necessary to have every subword of length 2 appear as a subword of \(\tilde{w}\). Instead, it is sufficient to use only the prefixes of the canonical representations of each necklace. For example, given the binary alphabet \(\{a, b\}\), every necklace has either \(aa, ab\) or \(bb\) as the prefix of length 2. Note that any necklace of length 2 followed by the largest symbol \(q\) in the alphabet \(n - 2\) times belongs to the set \(\mathcal{N}_{2s}^q\). As such, a simple lower bound on the number of prefixes of the canonical representation of necklaces is the number of necklaces of length 2, which in turn is bounded by \(\frac{q^2}{2}\). Noting that these prefixes in \(\tilde{S}\) may overlap, in order to ensure that \(\tilde{S}\) and \(\tilde{w}\) share at least one subword of length 2, the length of \(\tilde{S}\) must be at least \(\frac{q^2}{2}\). Similarly, for \(\tilde{S}\) and \(\tilde{w}\) to share \(i\) subwords of length 2, the length of \(\tilde{S}\) must be at least \(\frac{i \cdot q^2}{2}\). Hence the maximum number of subwords of length 2 that \(\tilde{S}\) and \(\tilde{w}\) can share is either \([\frac{2n \cdot k}{q^2}]\), if \([\frac{2n \cdot k}{q^2}] \leq n\), or \(n\) otherwise. More generally, in order for \(\tilde{S}\) to share at least one subword of length \(j\) with \(\tilde{w}\), the length of \(\tilde{S}\) must be at least \(\frac{j \cdot q^2}{2}\). Further the maximum number of subwords of length \(j\) that \(\tilde{S}\) and \(\tilde{w}\) can share is either \([\frac{j \cdot n \cdot k}{q^2}]\), if \([\frac{j \cdot n \cdot k}{q^2}] \leq n\), or \(n\) otherwise.

Using these observations, the maximum length of a common subword that \(\tilde{w}\) can share with \(\tilde{S}\) is the largest value \(l\) such that \(\frac{l \cdot q}{2} \leq n \cdot k\). By noting that \(\frac{l}{q} \geq \frac{q^2}{2}\), an upper bound on \(l\) can be derived by
rewriting the inequality \( \frac{q}{n} \leq n \cdot k \) as \( l = 2 \log_q (n \cdot k) \). Note further that, for any value \( l' > l \), there must be at least one necklace that does not share any subword of length \( l' \) with \( \mathbf{w} \) as \( \mathbf{w} \) cannot contain enough subwords to ensure that this is the case. This bound allows an upper bound number of shared subwords between \( \mathbf{w} \) and \( \mathbf{w} \) to be given by the summation \( \sum_{i=1}^{\log_q (n \cdot k)} \min(\lfloor \frac{1 \cdot n \cdot k}{q^i} \rfloor, n) \leq n \cdot \log_q (n \cdot k) + \frac{\log_q (n \cdot k)}{q-1} \approx \frac{q \cdot \log_q (k \cdot n)}{q-1} \approx n \log_q (k \cdot n) \). Using this bound, the distance between \( \mathbf{w} \) and \( \mathbf{w} \) must be no less than \( 1 - \frac{\log_q (k \cdot n)}{n} \).

The same arguments can be applied to the multidimensional case. Let \( \mathbf{m} = (m_1, m_2, \ldots, m_d) \) be a size vector of \( d \)-dimensions such that \( M = m_1 \cdot m_2 \cdot \ldots \cdot m_d \). The largest value of \( M \) such that \( \mathbf{w} \) can contain every subword with \( M \) positions is \( 2 \log_q (n \cdot k) \). The upper bound on the number of words of size \( \mathbf{w} \) is \( \frac{q^d}{M} \). Let \( F(x, \mathbf{m}) \) return the size of the set \([\mathbf{m}]\), i.e. the number of vectors with \( x \) positions that are less than or equal to \( \mathbf{m} \) in each dimension. Using this notation, the maximum number of shared subwords between \( \mathbf{w} \) and \( \mathbf{w} \) is \( \sum_{i=1}^{\log_q (n \cdot k)} \frac{M}{q} \cdot \frac{\log_q (k \cdot n)}{q-1} \). Note that \( \sum_{i=1}^{\log_q (n \cdot k)} \frac{M}{q} \cdot \frac{\log_q (k \cdot n)}{q-1} \leq \sum_{i=1}^{\log_q (n \cdot k)} \frac{\log_q (k \cdot n)}{q-1} \). Therefore, the upper bound on the number of common subwords in the multidimensional setting is \( N \log_q (k \cdot N) \), giving a bound on the distance of \( 1 - \frac{\log_q (k \cdot N)}{N} \).

Sections 8.2 provides an approximation algorithm for the \( k \)-centre problem using Lemma 15 as a lower bound. The first of these is \( 1 + (\frac{\log_q (k \cdot N)}{N} - \frac{\log_q (k \cdot N)}{N}) \)-approximate with a running time \( O(N \cdot k) \), but it requires access to the de-Bruijn hypertori of the multidimensional necklaces; this is a generalisation of de-Bruijn sequences. When \( d = 1 \), there exists an efficient algorithm for computing the de-Bruijn sequence. However, for \( d > 1 \), no algorithm is known for computing a de-Bruijn hypertori. Therefore, we develop a second algorithm that is \( 1 + (\frac{\log_q (k \cdot N)}{N} - \frac{\log_q (k \cdot N)}{N}) \)-approximation with a running time \( O(N^6) \), requiring techniques presented in Section 8.

The main idea behind both algorithms is to try to find the largest size vector \( \mathbf{v} = (l_1, l_2, \ldots, l_d) \) such that every subword of size \( \mathbf{v} \) appears at least once in some word within the set. In this setting \( \mathbf{m} \) is larger than \( \mathbf{v} \) if \( m_1 \cdot m_2 \cdot \ldots \cdot m_d > l_1 \cdot l_2 \cdot \ldots \cdot l_d \). This is motivated by observing that if two necklaces share a subword of length \( l \), they must also share \( 2 \) subwords of length \( l - 1 \), \( 3 \) of length \( l - 2 \), and so on. Lemma 16 provides an upper bound for the overlap distance between any necklace in \( \Sigma_q^N \) and the set \( \mathbf{w} \), containing all subwords of length \( l \).

**Lemma 16.** Given \( \mathbf{w}, \mathbf{v} \in \Sigma_q^N \) sharing a common subword \( \mathbf{a} \) of size \( \mathbf{m} \), let \( x_i = n_i \cdot m_i \) if \( n_i = m_i \), and \( x_i = \frac{m_i}{2} \) otherwise. The distance between \( \mathbf{w} \) and \( \mathbf{v} \) is bounded from above by \( \mathbf{D}(w, v) \leq 1 - \frac{\prod_{i=1}^{d} x_i}{N^2} \leq 1 - \frac{M^2}{N^2} \) where \( N = n_1 \cdot n_2 \cdot \ldots \cdot n_d \) and \( M = m_1 \cdot m_2 \cdot \ldots \cdot m_d \).

**Proof.** Note that the minimum intersection between \( \mathbf{w} \) and \( \mathbf{v} \) is the number of subwords of \( \mathbf{a} \), including the word \( \mathbf{a} \) itself. To compute the number of subwords of \( \mathbf{a} \), consider the number of subwords starting at some position \( j \in [\lfloor |\mathbf{a}| \rfloor] \). Assuming that \( |\mathbf{a}|_i < n_i \) for every \( i \in [d] \), the number of subwords starting at \( j \) corresponds to the size of the set \( [j, |\mathbf{a}|] \), equal to \( \prod_{i=1}^{d} m_i - |\mathbf{a}|_i \). This gives the number of shared subwords as being at least \( \sum_{j=\lfloor |\mathbf{a}| \rfloor}^{N} \prod_{i=1}^{d} m_i - |\mathbf{a}|_i \geq \sum_{j=\lfloor |\mathbf{a}| \rfloor}^{N} \prod_{i=1}^{d} m_i - \frac{M^2}{2} \). Therefore, the distance between \( \mathbf{w} \) and \( \mathbf{v} \) is no more than \( 1 - \frac{M^2}{2N^2} \). \( \square \)

### 8.2 Approximating the \( k \)-Centre Problem using de-Bruijn Sequences

In this section we provide our first approximation algorithm that requires access to de-Bruijn sequences for the 1D case and to de-Bruijn hypertori for higher dimensions. The main idea is to determine the largest de-Bruijn sequence that can fit into the set of \( k \)-centres. As the de Bruijn sequence of order \( l \) contains every word in \( \Sigma^l \) as a subword, by representing the de Bruijn sequence of order \( l \) in the set of centres we ensure that every necklace shares a subword of length \( l \) with the set of \( k \)-centres. Therefore, by determining the longest sequence that can be represented by \( k \) centres, an upper bound on the distance between the furthest necklace and the set of \( k \)-centres is derived.

**Definition 9.** A de Bruijn hypertorus of order \( \mathbf{n} \) is a cyclic \( d \)-dimensional word \( \bar{T} \) containing, as a subword, every word of size \( \mathbf{n} \) over the alphabet \( \Sigma \) of size \( q \). Further, such each word of size \( \mathbf{n} \) over the alphabet \( \Sigma \) appears exactly once as a subword of \( \bar{T} \).
Lemma 17. There exists an $O(n \cdot k)$ time algorithm for the $k$-Centre problem on $N_q^n$ such that every word in $N_q^n$ shares a common subword of length at least $\log_q(n \cdot k)$ with one or more centres. Further, no word in $N_q^n$ is at a distance of more than $1 - \frac{\log_q^2(n \cdot k)}{2n}$ from the nearest centre.

Proof. The high level idea of this algorithm is to split a de Bruijn sequence of order $\lambda$ between the $k$ centres. The motivation behind this approach is to represent every word of length $\lambda$ as a subword of at least one centre. Note that the length of the de Bruijn sequence of order $\lambda$ is $q^\lambda$.

Given a de Bruijn sequence $\bar{s}$, naively splitting $\bar{s}$ into $k$ words may lead to subwords being lost. For example, take the de Bruijn sequence of order 4 over the alphabet $\{a, b\}$ with subwords of length 8 results in the samples $aaabaaab$ and $bababbb$, missing the words $aabb, abba,$ and $bbab$. In order to account for this, the sequence is split into centres of size $n - \lambda + 1$, with the final $\lambda - 1$ symbols of the $i^{th}$ centre being shared with the $(i+1)^{th}$ centre. In this manner, the first centre is generated by taking the first $n$ symbols of the de Bruijin sequence. To ensure that every subword of length $\lambda$ occurs, the first $\lambda - 1$ symbols of the second centre is the same as the last $\lambda - 1$ symbol of the first centre. Repeating this, the $i^{th}$ centre is the subword of length $n$ starting at position $i(n - \lambda + 1) + 1$ in the de Bruijn sequence. An example of this is given in Figure 7.

The leaves the problem of determining the largest value of $\lambda$ such that $q^\lambda \leq k \cdot (n - \lambda + 1)$. The inequality $q^\lambda \leq k \cdot (n - \lambda + 1)$ can be rearranged in terms of $\lambda$ as $\lambda \leq \log_q(k \cdot (n + 1) - k \cdot \lambda)$. Noting that $\lambda$ must be no more than $\log_q(k \cdot n)$, this upper bound on the value of $\lambda$ can be rewritten as $\log_q(k \cdot (n + 1 - \log_q(k \cdot n))) \approx \log_q(k \cdot n)$. Using Lemma 16 along with $\log_q(k \cdot n)$ as an approximate value of $\lambda$ gives an upper bound on the distance between each necklace in $N_q^n$ and the set of samples of $1 - \frac{\log_q^2(n \cdot k)}{2n}$.

As the corresponding de Bruijin sequence can be computed in no more than $O(k \cdot n)$ time [52] and the set of samples can be further derived from the sequence in at most $O(k \cdot n)$ time, the total complexity is at most $O(k \cdot n)$. Note that any algorithm that outputs such a set of centres takes at most $\Omega(k \cdot n)$ time.

Theorem 9. The $k$-centre problem for $N_q^n$ can be approximated in $O(n \cdot k)$ time with an approximation factor of $1 + f(n,k)$ where $f(n,k) = \frac{\log_q(k \cdot n)}{n - \log_q(k \cdot n)} - \frac{\log_q^2(n \cdot k)}{2n(n - \log_q(k \cdot n))}$ and $f(n,k) \rightarrow 0$ for $n \rightarrow \infty$.

Proof. Recall from Lemma 15 that the overlap distance is bounded by $1 - \frac{\log_q^2(n \cdot k)}{2n}$. Using the lower bound of $1 - \frac{\log_q^2(n \cdot k)}{2n}$ given by Lemma 17 gives an approximation ratio of $1 - \frac{\log_q^2(n \cdot k)}{2n} = \frac{2n - 2 \log_q^2(n \cdot k)}{2n^2 - 2 \log_q^2(n \cdot k)} = 1 + \frac{\log_q^2(n \cdot k)}{2n(n - \log_q(k \cdot n))}$. Note that $f(n,k) = \frac{2n \log_q^2(n \cdot k) - \log_q^2(n \cdot k)}{2n^2 - 2 \log_q^2(n \cdot k)}$ converges to 0 when $n \rightarrow \infty$ for a constant $k < q^n/n$.

Theorem 10. Let $T$ be a $d$-dimensional de Bruijin hyper torus of size $(x, x, \ldots, x)$. There exist $k$ subwords of $T$ that form a solution to the $k$-centre problem for $N_q^{(d)}$ with an approximation factor of $1 + f(n,k)$ where $f(n,k) = \frac{\log_q(k \cdot N)}{N - \log_q(k \cdot N)} - \frac{\log_q^2(k \cdot N)}{2N(N - \log_q(k \cdot N))]}, f(n,k) \rightarrow 0, N \rightarrow \infty$.

Proof. Recall from Lemma 15 that the lower bound on the distance between the centre and every necklace in $N_q^n$ is $1 - \frac{\log_q(k \cdot N)}{N}$. As in Theorem 9, the goal is to find the largest de Bruijin torus that can “fit” into the centres. To simplify the reasoning, the de Bruijin hyper tori here is limited to those corresponding to the word where the length of each dimension is the same. Formally, the de Bruijin hypertori are restricted to be of the size $m_1 = m_2 = \ldots = m_d = \sqrt{N}$ for some $j \in [d]$, giving the total number of positions in the tori as $M$. Similarly, the centres are assumed to have size $n_1 = n_2 = \ldots = n_d = \sqrt{N}$, giving $N$ total positions.

Observe that the largest torus that can be represented in the set of centres has $M$ positions such that $q^M \leq k \cdot N^{(d-j)}/d^{(\sqrt{N} - \sqrt{M} + 1)}$. This can be rewritten to give $M \leq \log_q(k \cdot N^{(d-j)}/(d^{(\sqrt{N} - \sqrt{M} + 1)})$. Noting that $M$ is of logarithmic size relative to $N$, this is approximately equal to $M \leq \log_q(k \cdot N)$. Using Lemma 16, the minimum distance between any necklace in $N_q^n$ is $1 - \frac{\log_q^2(k \cdot N)}{2N}$. This is compared to the optimal solution, following the arguments from Theorem 9 giving a ratio of $1 + f(N,k)$ where $f(N,k) = \frac{2N \log_q^2(k \cdot N) - \log_q^2(k \cdot N)}{2N^2 - 2N \log_q^2(k \cdot N)} = \frac{\log_q(k \cdot N)}{N - \log_q(k \cdot N)} - \frac{\log_q^2(k \cdot N)}{2N(N - \log_q(k \cdot N))]}. \square$

For both cases table providing some explicit examples of the approximation ratio for different values of $n$ and $k$ is given in Table 1. While this provides a good starting point for solving the $k$-Centre problem for
inequality set $S$ assume without loss of generality that $q$ samples, each of which can be made into a word of size $\log k$ for a binary alphabet (top) and an alphabet of size 8 (below). Note that when $k \geq q^n$ the approximation ratio is 1 as every necklace can be represented in the set.

$N_{k^n}$ results on generating de Bruijn tori are highly limited, focusing on the cases with small dimensions 7, 27, 29, 30, 31. As such an alternate approach is needed.

Theorem 11 presents such an alternate approach. At a high level, the idea is to reduce the problem from the multidimensional setting to the 1D problem which we can already solve. Given a size vector $n$, integer $k$ and alphabet $\Sigma$, this approach can be thought of as finding a set of $k \cdot n_1 \ldots n_{d-1}$ samples of length $n_d$ over $\Sigma$, taking advantage of the added number of samples to increase the lower bound on the length of shared subwords. There are two cases to consider based on the values of $n$.

Case 1, $q^{n_d} \leq k \cdot \frac{N}{n_d}$: In this case the set of samples is constructed by using $k' = \frac{kN}{n_d}$ samples of $N_{q^{n_d}}$. The motivation behind this approach is to optimise the length of the 1D subwords that are shared by the sample and every other necklace in $N_{q^{n_d}}$. Let $S \subseteq N_{q^{n_d}}$ be a set of samples $k \cdot \frac{N}{n_d}$ from $N_{q^{n_d}}$ constructed following the algorithm outline in Lemma 17. Following the arguments from Lemma 17 every necklace in $N_{q^{n_d}}$ must share a subword of length $\log_q(k \cdot N)$ with at least one sample in $S$. As every subword of size $(1, 1, \ldots, 1, n_d)$ of any necklace in $N_{q^{n_d}}$ belongs to a necklace $w \in N_{q^{n_d}}$, by ensuring that every necklace in $S$ appears as a subword in the sample $S' \subseteq N_{q^{n_d}}$ it is ensured that $w$ shares at least one subword of length $\log_q(k \cdot N)$ with some necklace in $S'$. This can be done by simply splitting $S$ into $k$ sets of $\frac{N}{n_d}$ samples, each of which can be made into a word of size $n$ through concatenation. From Lemma 16 the maximum distance between any necklace in $S'$ and necklace in $N_{q^{n_d}}$ is $1 - \frac{\log_q(k \cdot N)}{2N \cdot n_d}$. Note that this is equal to the bound given by Lemma 17, resulting in the same approximation ratio.

Case 2, $q^{n_d} > k \cdot \frac{N}{n_d}$: In this case, following the process outlined above, it is possible to represent every word of length $n_d$ over $\Sigma$ with some redundancy. In order to make better use of the samples, and reduce the redundancy, an alternative reduction from the 1D setting is constructed. The high level idea is to construct a new alphabet such that each symbol corresponds to some word in $\Sigma^{n_d}$ for some size vector $m$.

The first problem becomes determining the size vector such that this reduction can be done. Let $\Sigma(m)$ denote the alphabet of size $q^{m_1 \cdot m_2 \ldots m_d}$ such that each symbol in $\Sigma(m)$ corresponds to some word in $\Sigma^{n_d}$. Given a word $\hat{w} \in \Sigma(m)^{m_1/m_2/m_3\ldots/m_d}$ a word $\hat{v} \in \Sigma^{n_d}$ can be constructed by replacing each symbol in $\hat{w}$ with the corresponding symbol in $\Sigma^{n_d}$. Note that the largest value of $m$ such that every symbol in $\Sigma(m)$ can be represented in $k$ words from $\Sigma(m)^{m_1/m_2/m_3\ldots/m_d}$ is bounded by the inequality $q^{m_1 \cdot m_2 \ldots m_d} \leq k \cdot \frac{m_1}{m_2} \cdot \frac{m_2}{m_3} \ldots \frac{m_d}{m_{d-1}}$. Letting $M = m_1 \cdot m_2 \ldots m_d$, this inequality can be rewritten as approximately $q^{M} \leq k \cdot \frac{N}{m}$. Treating $M$ as being approximately $N$ for the purpose of giving an upper bound to $M$ gives $M \leq \log_q(k)$.

Using this bound on $M$ let $m$ be some set of vectors such that $M = m_1 \cdot m_2 \ldots m_d$. We may assume without loss of generality that $m_d = 1$. The samples for $N_{q^{n_d}}$ are constructed by making a set $S$ of $k \cdot \frac{N}{m_1 \cdot m_2 \ldots m_{d-1}}$ samples for $N_{q^{n_d}}$. Following the arguments from Lemma 17 every necklace in $N_{q^{n_d}}$
must share a subword of length at least \( \log_q(k \cdot N) = \log_q(k \cdot \frac{N}{m^{\alpha}}) = \frac{\log_q(k \cdot \frac{N}{m^{\alpha}})}{\log_q(k)} \). Note further that, as each symbol in \( \Sigma(m) \) corresponds to a word in \( \Sigma(m) \), converting each word in \( S \) to a word of size \( (m_1, m_2, \ldots, m_{d-1}, n_1) \) provides a sample such that every necklace in \( \mathcal{N}_q(m_1, m_2, \ldots, m_{d-1}, n_1) \) shares a subword of size \( (m_1, m_2, \ldots, m_{d-1}) \), \( \frac{\log_q(k \cdot \frac{N}{m^{\alpha}})}{\log_q(k)} \) with some member of the sample. Converting this new sample into a sample \( S' \subseteq \mathcal{N}_q(m) \) maintains the same size of shared subwords. From Lemma 16, the furthest distance between \( S' \) and any necklace in \( \mathcal{N}_q(m) \) is bounded from above by \( 1 - \frac{\log_q(k) \cdot \frac{\log_q(k)}{\log_q(k)}}{2N^2} \).

**Theorem 11.** The \( k \)-centre problem for \( \mathcal{N}_q(m) \) can be approximated in \( O(N^2k) \) time within an approximation factor of \( 1 + \frac{\log_q(k)}{N - \log_q(kN)} - \frac{\log_q(k)}{2N(N - \log_q(kN))} \), where \( N = \prod_{i=1}^{d} n_i \).

**Proof.** Following the above construction, note that in both cases the algorithm bounds the upper distance between samples by approximately \( 1 - \frac{\log_q(k)}{N - \log_q(kN)} \). Following the same arguments as in Theorem 9 gives the approximation ratio of \( 1 + \frac{\log_q(k)}{N - \log_q(kN)} - \frac{\log_q(k)}{2N(N - \log_q(kN))} \). Regarding time complexity, in the first case the problem can be solved in \( O(k \cdot N) \) time using Theorem 9. In the second case, a brute force approach to find to best value of \( m \) can be done in \( O(N) \) additional time steps giving a total complexity of \( O(k \cdot N^2) \). \( \square \)

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