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ICE-TCS
Icelandic Centre of Excellence
in Theoretical Computer Science

The k-centre problem for necklaces

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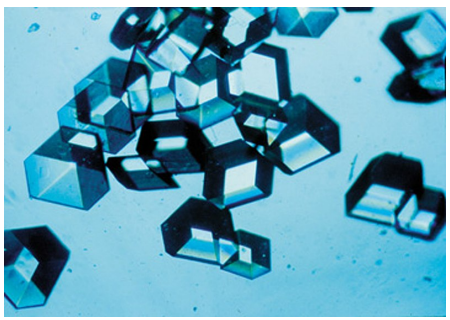
Why Crystals?

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

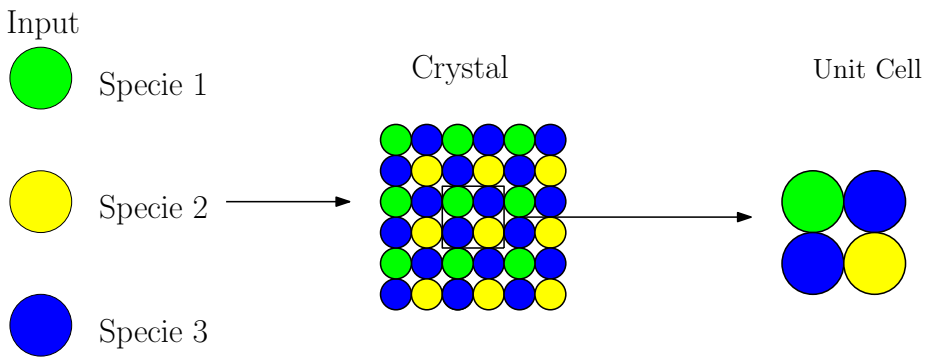
Crystals are everywhere

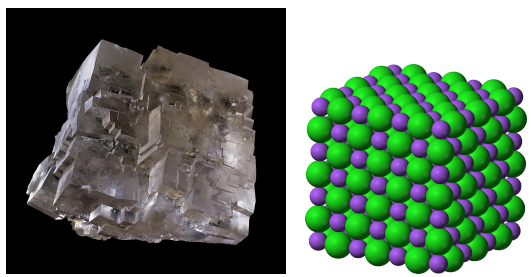


Crystals

Definition (Crystals)

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

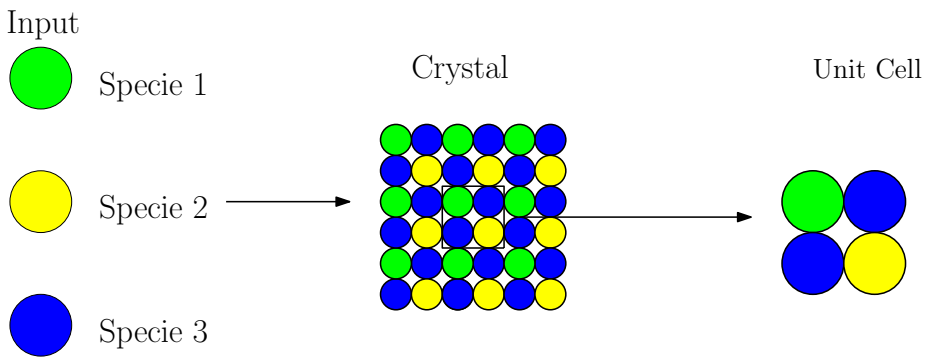


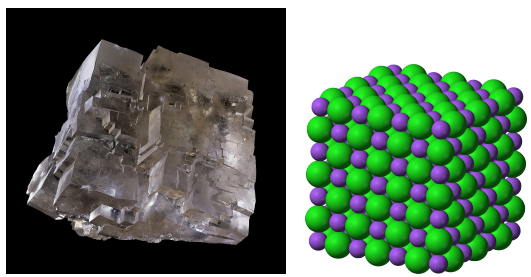


Crystals

Definition (Unit Cells)

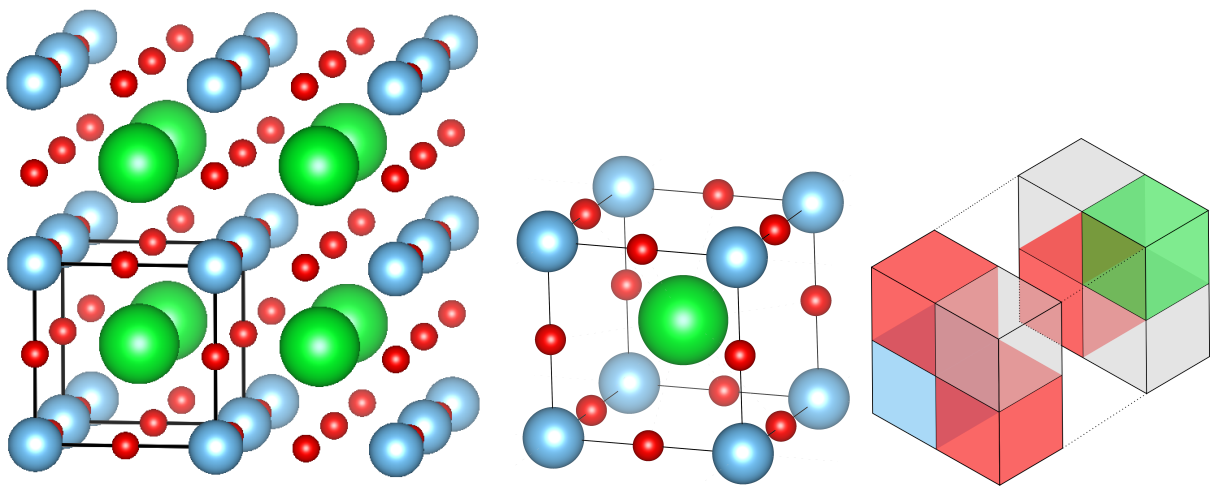
A **Unit Cell** is a contiguous region of space containing some set of **Ions**.





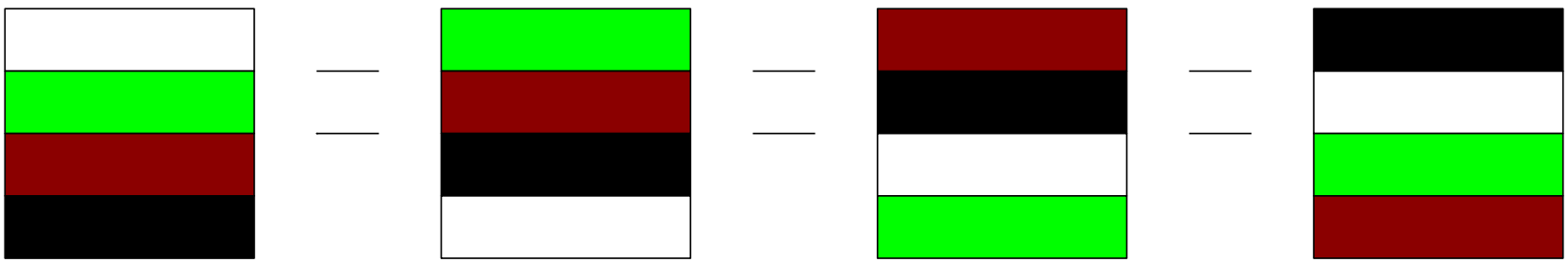
Discrete Crystals

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



1D Crystals

- In this talk we are going to focus on **1D-Crystals**[1].
- These can be thought of a crystals made from precomputed 3D-blocks, with a high degree of symmetry along two dimensions.
- The main challenge in **uniquely** representing these structures is capturing **translational symmetry**.



[1] C. Collins et al. "Accelerated discovery of two crystal structure types in a complex inorganic phase field". In: *Nature* 546.7657 (2017), p. 280.

Goal

Select a **representative** set of crystal structures from the set of all possible structures of a given size over a given alphabet of "blocks".

Problems

Question

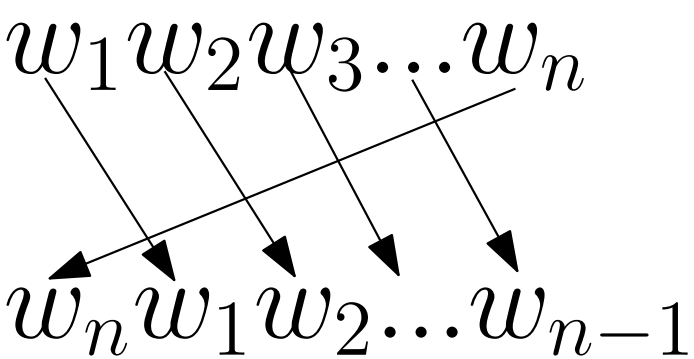
How can we represent crystals **uniquely***?*

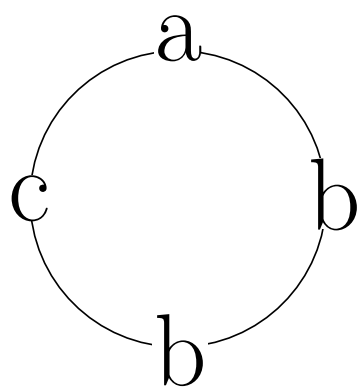
Question

How can we choose a **representative sample** *from this representation?*

Necklaces

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





abbc
bbca
bcab
cabb

Some Notation for 1D Necklaces

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

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

Representative Samples

- To get a set of **representative crystals**, we want to choose a set of crystals that contain as many **local structures** as possible, in order understand the global energy space.
- As energy interaction is strongest at close range, by analysing local structures we can get a good idea about the full energy space.

Question

How do formalise this as a mathematical problem?

Finding Representative Samples

- In order to find a set of representative samples, we turn to the **k-centre problem**.
- Informally, the k-centre problem asks us to select a set k vertices from a graph $G = (V, E)$ minimising the function:

$$\min_{S \subseteq_k V} \max_{v \in V} \min_{s \in S} D(s, v)$$

- Where S is a set of k vertices from V, and $D(s, v)$ is the distance between some pair of vertices in G.

Question

How can we measure the distance between necklaces?

The Overlap Distance for Necklaces

- Following our motivation of comparing **crystal structures**, we need to define a distance that represents structures with similar properties.
- As much of the energy in crystaline structures is due to **local** interactions, we use the number of **shared subwords** as a basis for measuring the similarity.

Definition

The **overlap distance** between two necklaces $\tilde{\mathbf{w}}$ and $\tilde{\mathbf{u}}$ is defined as the number of shared subwords between $\tilde{\mathbf{w}}$ and $\tilde{\mathbf{u}}$, normalised by the total number of subwords.

The Overlap Distance for Necklaces

	word $abab$	word $aabb$	Intersection
1	$a \times 2, b \times 2$	$a \times 2, b \times 2$	
2	$ab \times 2, ba \times 2$	$aa \times 1$ $ab \times 1$, $bb \times 1, ba \times 1$	
3	$aba \times 2, bab \times 2$	$aab \times 1, abb \times 1$, $bba \times 1, baa \times 1$	
4	$abab \times 2, baba \times 2$	$aabb \times 1, abba \times 1$, $bbaa \times 1, baab \times 1$	
$\mathfrak{D}$			?/16

The Overlap Distance for Necklaces

	$abab$	$aabb$	Intersection
1	$\mathbf{a} \times 2, \mathbf{b} \times 2$	$\mathbf{a} \times 2, \mathbf{b} \times 2$	4
2	$\mathbf{ab} \times 2, \mathbf{ba} \times 2$	$aa \times 1$ $\mathbf{ab} \times 1$, $bb \times 1, \mathbf{ba} \times 1$	2
3	$aba \times 2, bab \times 2$	$aab \times 1, abb \times 1$, $bba \times 1, baa \times 1$	0
4	$abab \times 2, baba \times 2$	$aabb \times 1, abba \times 1$, $bbaa \times 1, baab \times 1$	0
$\mathfrak{D}$			6/16

Challenges

- There are $O(q^n)$ necklaces in $\mathcal{N}_q^n$, so explicitly representing the graph is not feasible even for moderate values of n.
- Trying to determine the properties of a necklace as a crystal structure is computationally expensive.
- The graph is highly structured, with some vertices being much better than others.

Our Approach

- Our goal is to select a set of k-centres **maximising** the number of **distinct subwords** that appear in any centre.
- We do this by finding the longest length λ for which every word in Σ^λ can appear at least once in the set of centres.

Observation

Let $S \subseteq_k \mathcal{N}_q^n$ be a set of k necklaces such that every word in Σ^λ appears as a subword in at least one necklace in S. Then, every necklace in $\mathcal{N}_q^n$ is at most $\frac{\lambda^2}{n}$ from the nearest centre in S.

de-Bruijn Sequences

Definition

The **de-Bruijn Graph** of order m over a k-ary alphabet Σ is a directed graph of k^m vertices where each vertex corresponds uniquely to some word in Σ^m. There exists an edge from v to u if and only if $v : u_m = v_1 : u$.

Definition

A **de-Bruijn Sequence** of order m over a k-ary alphabet Σ is a cyclic word w of length k^m such that every word in Σ^m appears exactly once in w. In other words, w corresponds to a Hamiltonian circuit on the de-Bruijn graph.

Example of the de-Bruijn graph and sequence

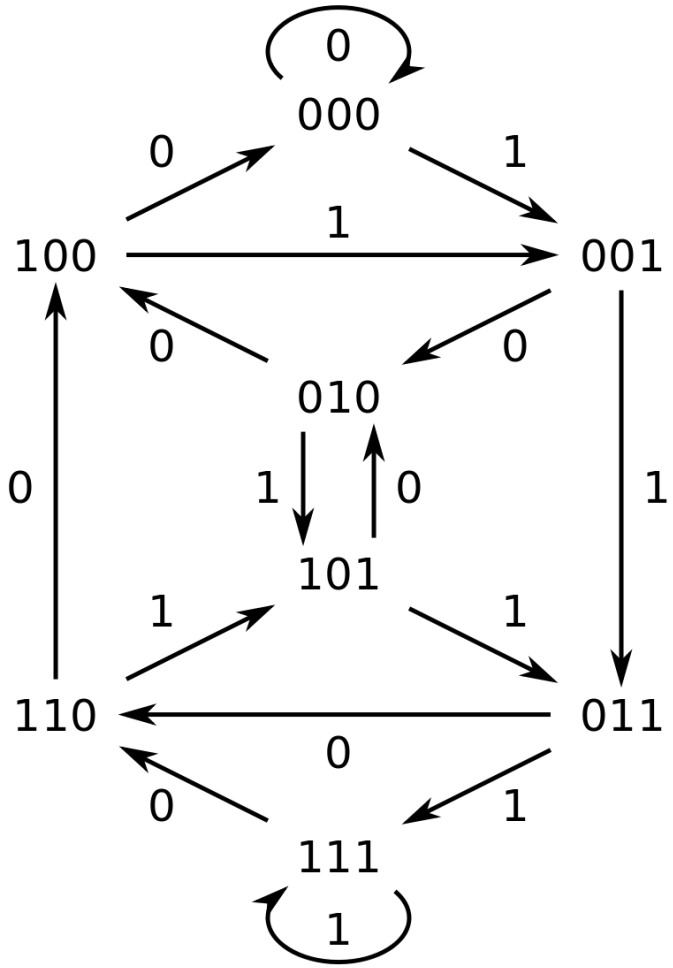


Figure 1: 00010111

de-Bruijn Sequences

- **De-Bruijn Sequences** are a classic combinatorial object.
- There are strong results for generating[2] and decomposing[3].

[2] Fred S. Annexstein. "Generating de Bruijn sequences: An efficient implementation". In: *IEEE Transactions on Computers* 46.2 (1997), pp. 198–200.

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

de-Bruijn Sequences

- **De-Bruijn Sequences** are a classic combinatorial object.
- There are strong results for generating[2] and decomposing[3].
- **Idea**. We can use de-Bruijn sequences as a basis to compute a set of centres.

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One Centre

- When $k = 1$, centre can be computed by finding the largest value of λ for which $q^\lambda \leq n$, giving $\lambda = \lfloor \log_q n \rfloor$.
- This ensures that every word of length λ appears at least once in the centre.

Claim

When $k = 1$, this process returns the optimal centre.

Multiple Centres

- When $k > 1$, a slightly more sophisticated approach is needed.
- The main challenge is determining how to **partition** the de-Bruijn sequence.

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- The main challenge is determining how to **partition** the de-Bruijn sequence.
- **Idea**. we need to build some redundancy to the centres.

Multiple Centres

Sequence:	00000100011001010011101011011111
Centre	Word
1	00000100 0110
2	01100101 0011
3	00111010 1101
4	11011111 0000

Figure 2: Example of how to split the de Bruijn sequence of order 5 between 4 centres. Highlighted parts are the shared subwords between two centres.

Multiple Centres

Claim

The k-centre problem for $\mathcal{N}_q^n$ *can be approximated in* $O(n \cdot k)$ *time with an approximation factor of* $1 + \frac{\log_q(k \cdot n)}{n - \log_q(k \cdot n)} - \frac{\log_q^2(k \cdot n)}{2n(n - \log_q(k \cdot n))}$.

Online Centre Selection

- In practice, it is useful to have a tool that allows us to add more centres after the initial set have been analysed.
- To solve this we turn to the **online k-centre selection** problem.

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- To solve this we turn to the **online k-centre selection** problem.
- **Assumptions**:
  - Every centre that has already been chosen is **fixed**.
  - We do not know at the start how many centres are needed.

Solving the Online Centre Selection

- The first centre corresponds to the de-Bruijn sequence of length $\lfloor \log_q n \rfloor$.
- The next q centres correspond to the de-Bruijn sequence of length $\lfloor \log_q n \rfloor + 1$.
- The $q^j + i^{th}$ centre corresponds to the i^{th} "centre" needed to cover the de-Bruijn sequence of order $j + 1$.
- This results in an algorithm that is at most a factor of 2 worse the than offline version.

Covering the de-Bruijn Graph

Question

Given an integer $l > m$, what is the smallest number j of length l cycles needed to cover the k-ary de-Bruijn graph of order m?

Paritial Results

- Some experimental evaluation suggests that, in general, we need $O(\frac{k^m}{l})$ cycles. And normally we only need $\frac{k^m}{l} + 1$.

de Bruijn (Hyper) Torus

- The same ideas from the 1D setting can be applied to the multidimensional setting, however doing so requires the ability to generate **de Bruijn tori** (the multidimensional analogue of the de Bruijn sequence).
- At present, we can approximate the de-Bruijn torus for any dimension, however this comes at the cost of slight less precision.
- **High Level Idea.** We treat each word of size $n_1 \times n_2 \times \cdots \times n_d$ as $n_2 \cdot n_3 \cdot \cdots \cdot n_d$ 1D-words of size n_1.