# SageMath package for finding growth functions of periodic tessellation

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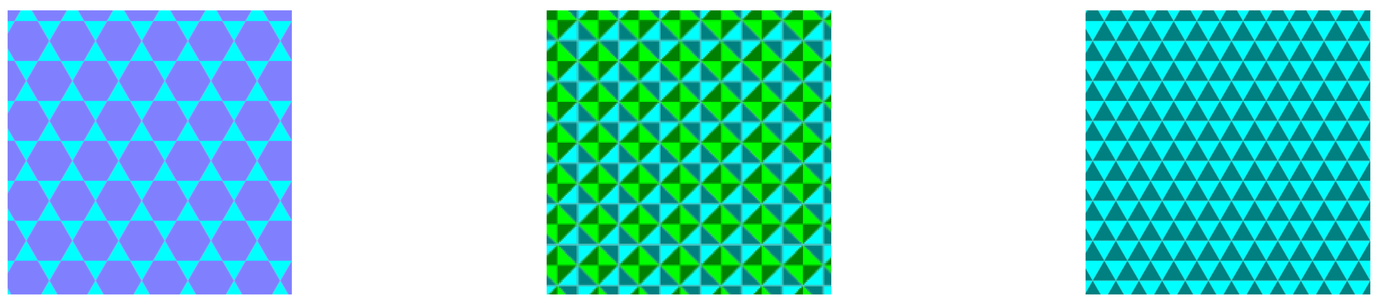
## Introduction

Crystal structure can be treated as tessellation of the Euclidean space. We investigate relative growth functions of periodic tessellations and expect that such data might be enough to encode tessellation's space group or even the whole information about tessellation. As part of the ongoing project SageMath package dedicated to the growth functions has been created.

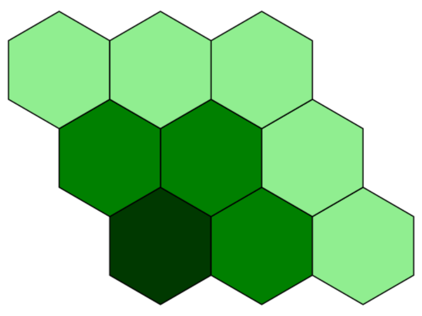


## Topological growth functions

For every periodic tessellation of $\mathbb{R}^N$ there exist motif $\Omega$ and set of vectors $\{v_i\}_{i=1}^N$ such that we can construct this tessellation by translating the motif by vectors from the set. We can approximate tessellation by sequence $(\mathcal{T}_n)$, where

$$\mathcal{T}_n = \bigcup_{\mathrm{m}\in[n]^N} \left\{ \Omega + \sum_{i=1}^{N} m_i v_i \right\}.$$

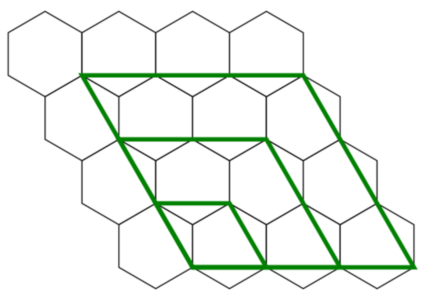
The topological growth function counts the number of tessellation elements (vertices, edges, fields) in $\mathcal{T}_n$.



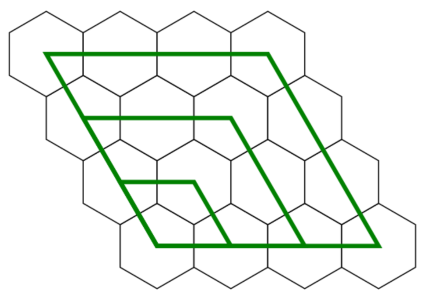
$$f_0(n) = 2n^2 + 4n$$
$$f_1(n) = 3n^2 + 4n - 1$$
$$f_2(n) = n^2$$

## Crystallographic growth functions

Crystallographic growths functions measure the growth of tessellation against the propagation of the unit cell which is a parallelogram with a fixed anchor point. As you can see on examples below, these functions are sensitive to the choice of the anchor point.

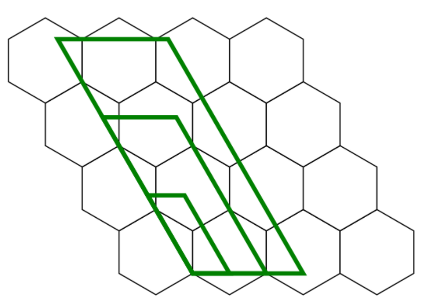


$$f_0(n) = 2n^2 + 2n + 1$$
$$f_1(n) = 3n^2$$
$$f_2(n) = n^2 - 2n + 1$$



$$f_0(n) = 2n^2$$
$$f_1(n) = 3n^2 - 2n$$
$$f_2(n) = n^2 - 2n + 1$$

Scaling the sides of the frame by rational numbers complicates the form of the growth function, however such functions can also be found by our package.



Example of modified frames
Scaling values: $\frac{1}{2}$ and $\frac{11}{9}$

## How to find the functions

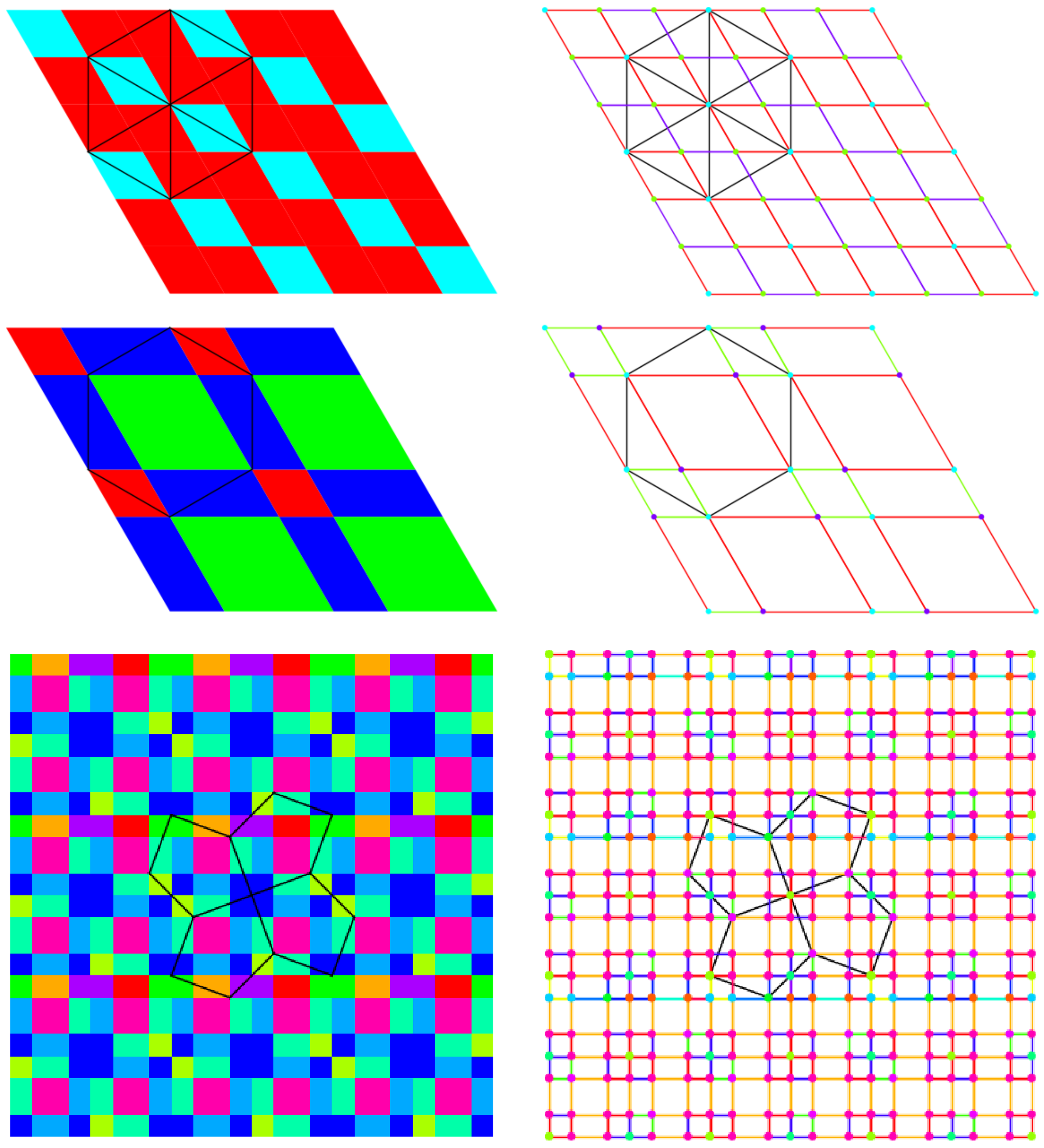
Growth function of periodic tessellation can be described using polynomials. The package finds their coefficients by solving systems of linear equations.

$$\begin{cases} f_0(1) = \phantom{4}a_2 + \phantom{2}a_1 + a_0 \\ f_0(2) = 4a_2 + 2a_1 + a_0 \\ f_0(3) = 9a_2 + 3a_1 + a_0 \end{cases}$$

In case of modified frames number of polynomials, that need to be found, is equal to the least common denominator of scaling values.

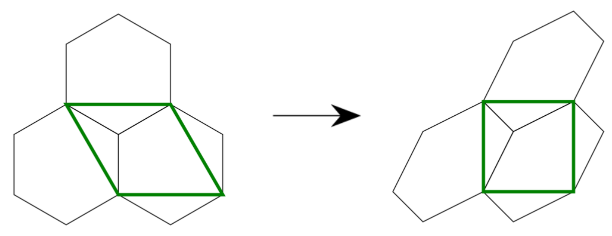
## Tessellation diagrams

The package allows to visualize how crystallographic growth functions depend on anchor point. Anchor points can be grouped into regions within which the growth functions are identical. Every colour on diagrams below represents different triple of growth functions.



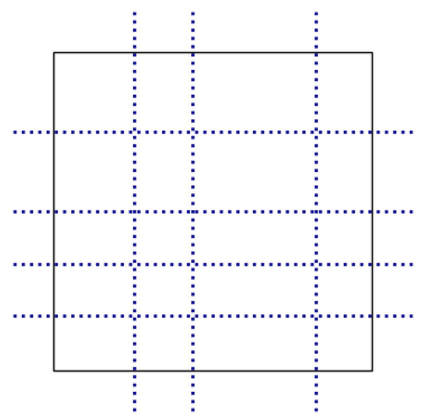
## How to find the regions

When looking for the regions with identical growth functions, it is convenient to use crystallographic coordinates. When applied, the frames are square and points' coordinates can be analysed independently.



If, despite the shifting of frames, the set of vertices contained in them has not changed, then the growth functions also remains the same. To check how much we can move the frame so that the given vertex is still inside/outside the frame, we subtract from its coordinates the anchor point's coordinates and analyse result's mantissas.

Applying this method on a subset of tessellation vertices, we first move along one axis and then along the other and we find lines that determine the regions we are looking for.



## Package's details

The results returned by the package are exact. Numerical errors are eliminated by using symbolic calculations. Current implementation works only for 2-dimensional tessellations, but we are developing a version of this package which will work in dimensions 3 and beyond.

You can find the package here

https://github.com/Malinon/crystgrowthfunctions

## References

[1] B. Naskrecki, Z. Dauter and M. Jaskolski A topological proof of the modified Euler characteristic based on the orbifold concept. *Acta Crystallographica Section A, 77(4):317–326, Jul 2021.*