The Messthaler-Wulff Project

Blazingly fast code for finding all crystals (subsets of a graph) that can be constructed using only transformations that locally minimize surface energy.

The Problem

Let G be some graph and $C \subset G$ a crystal. Furthermore let $\eta : G \to \wp(G)$ denote the neighbors of a given node. Then we can define the surface energy of the crystal C as

$$\xi_C \coloneqq \sum_{n \in C} l_n$$

where l_n denotes the loneliness of the node n and is itself defined as

$$l_n \coloneqq \#\{n_0 \in \eta(n) \mid n_0 \notin C\}$$

The idea now is to find optimal ξ_C by doing locally minimizing transformations. We call a node n optimal in forwards mode if for the specific C there is no node n_0 such that $l_{n_0} < l_n$. The same definition can be applied to backwards mode, for this however we use $\bar{l}_n \coloneqq \#\{n_0 \in \eta(n) \mid n_0 \in C\}$.

A locally optimal addition is now simply a node with optimal l_n and a locally optimal removal is a node with optimal $\bar{l}_n$.

Our goal in this project is to explore what crystals we can construct by only using such locally optimal transformations.

The Additive Simulation

This class encapsulates a current state representing a crystal and methods to find out what locally optimal transformations can be applied or to apply said transformations. It is optimized to be able to support $O(1)$ operations. A simplified definition of an additive simulation instance is $S_A = (\xi_C, B_0, B_1)$ where ξ_C is the energy of the current crystal and B_i are the boundaries, defined as follows:

$$B_0 = \{n \in C \mid l_n > 0\}$$

$$B_1 = \{n \notin C \mid \bar{l}_n > 0\}$$