1 preliminaries

Let Σ be a set of bead types, and Σ^* be the set of finite strings of beads. Let $w = a_1, ..., a_n$ be a string of length n for some integer n and bead types $a_1, ..., a_n \in \Sigma$. The *length* of w is denoted by $|w|$. For two indices i, j with $1 \leq i \leq j \leq n$, we let $w[i, j]$ refer to the substring $a_i a_{i+1} \cdots a_{j-1} a_j$. if $i = j$, then we express $w[i, i]$ as $w[i]$.

Oritatami systems operate on the hexagonal lattice. The *grid graph* (V, E) of the lattice is the graph whose vertexes correspond to the lattice points and connected if the corresponding lattice points are at unit distance hexagonally. a *path* in the grid graph is a sequence $P = p_1 p_2 \cdots p_n$ of *pairwise-distinct* points $p_1, p_2, \cdots, p_n \in V$ such that $p_i, p_{i+1} \in E$ for all $1 \leq i \leq n$.

Let $\mathcal{H} \subseteq \Sigma \times \Sigma$ be a symmetric relation, specifying between which types of beads can form a hydrogen-bond-based interaction (h-interaction for short). This is called the *ruleset*. It is convenient to assume a special *inert* bead type $\bullet \in \Sigma$ that never forms any h-interaction according to $\mathcal{H}$.

A *conformation* C is a triple of a *path* $P = p_1 p_2 \cdots p_n$ and a *word* w of length n, and set H of h-interaction, where $H \subseteq \{\{i, j\} | 1 \leq i, i+2 \leq j\}$ and $\{i, j\} \in H$ implies that the i-th and j-th beads of the path, i.e., p_i and p_j, form an h-interaction between them. The condition $i + 2 \leq j$ represents the topological restriction that two beads next to each other along the path can not form an h-interaction between them. From now on, when a conformation is illustrated, any unlabeled bead is assumed to be labeled with $\bullet$, that is, be inert. For an integer $\alpha \geq 1$, let $\mathcal{C}_\alpha$ be the set of all conformations of arity-α.

A rule (a, b) in the ruleset $\mathcal{H}$ is *used* in the conformation C if there exists $\{i, j\} \in H$ such that $w[i] = a$ and $w[j] = b$ or $w[i] = b$ and $w[j] = a$. A conformation C is *valid (with respect to $\mathcal{H}$)* if for all $\{i, j\} \in H, (w[i], w[j]) \in \mathcal{H}$. In a context with one fixed ruleset, only valid conformations with respect to the ruleset are considered, and we may not specify with respect to what ruleset they are valid.

Given a ruleset $\mathcal{H}$ and valid finite conformation $C_1 = (P, w, H)$ with respect to $\mathcal{H}$, we say that another conformation C_2 is an *elongation of C_1 by a bead $a \in \Sigma$* if $C_2 = (P \cdot p, w \cdot a, H \cup H')$ for some lattice point p not along the path P and (possibly empty) set of h-interactions $H' \subseteq \big\{\{i, |w|+1\} \mid 1 \leq i \leq |w|, (w[i], a) \in \mathcal{H}\big\}$. Note that C_2 is also valid. For a conformation C and finite string $w \in \Sigma^*$, we denote the set of all elongations of C by w, as $C_1 \xrightarrow{\mathcal{H}}_w C_2$.

1.1 Oritatami system

An *Oritatami system* is a 5-tuple $\Xi = (\mathcal{H}, \alpha, \delta, \sigma, w)$, where $\mathcal{H}$ is a *ruleset*, α is an *arity*, $\delta \geq 1$ is a parameter called the *delay*, σ is an initial valid conformation of arity α called the *seed*, upon which its *transcript* $w \in \Sigma^* \cup \Sigma^w$ is to be folded by stabilizing beads of$w$ one at a time so as to minimize energy collaboratively with the succeeding $\delta{-}1$ nascent beads. The energy of a conformation $C = [(P, w, H)]$, denoted by $\Delta G(C)$, is defined to be $-|H|$; the more h-interactions a conformation has, the more stable it gets. The set $\mathcal{F}(\Xi)$ of conformations *foldable* by this system is recursively defined as: the seed σ is in $\mathcal{F}(\Xi)$; and provided that an elongation C_i of σ by the prefix $w[1...i]$ be foldable (i.e., $C_0 = \sigma$), its further elongation C_{i+1} by the next bead $w[i+1]$ is foldable if

$$C_{i+1} \in \mathop{\arg\min}_{\substack{C \in \mathcal{C}_{\leq\alpha} s.t. \\ C_i \xrightarrow{\mathcal{H}}_{w[i+1]} C}} \min \left\{ \Delta G(C') \mid C \xrightarrow{\mathcal{H}^*}_{w[i+2...i+k]} C', k \leq \delta, C' \in \mathcal{C}_{\leq\alpha} \right\}. \quad (1)$$

We say that the bead $w[i+1]$ and the h-interactions it forms are *stabilized* according to C_{i+1}. Note that an arity-α oritatami system cannot fold any conformation of arity larger than α. A conformation foldable by Ξ is *terminal* if none of its elongations is foldable by Ξ. The set of all terminal conformations foldable by Ξ is denoted by $\mathcal{F}_\square(\Xi)$.

The oritatami system Ξ is *deterministic* if for all $i \geq 0$, there exits at most one C_{i+1} that satisfies (1). Thus, a deterministic oritatami system folds into a unique terminal conformation. The uniqueness is also a sufficient condition for an oritatami system to be deterministic because any foldable conformation can be elongated to a terminal foldable conformation.