[★] Exercise 1 (Building shapes with Oritatami). In this exercise, we will build shapes using the Oritatami co-transcriptional folding model. We will show that as opposed to tile assembly systems, Oritatami systems only need a small constant upscaling to build any shape.

Triangular lattice. Consider the triangular lattice defined as $\mathbb{T} = (\mathbb{Z}^2, \sim)$, where $(x, y) \sim (u, v)$ if and only if $(u, v) \in \bigcup_{\varepsilon = \pm 1} \{(x + \varepsilon, y), (x, y + \varepsilon), (x + \varepsilon, y + \varepsilon)\}$. Every position $(x, y)$ in $\mathbb{T}$ is mapped in the euclidean plane to $x \cdot X + y \cdot Y$ using the vector basis $X = (1, 0)$ and $Y = \text{RotateClockwise}(X, 120^\circ) = \left(-\frac{1}{2}, -\frac{\sqrt{3}}{2}\right) = \sqrt{3}$.

Oritatami systems. Let $B$ denote a finite set of bead types. Recall that an Oritatami system $\mathcal{O} = (p, \bowtie, \delta)$ is composed of:

1. a bead type sequence $p \in B^*$, called the primary structure;
2. an attraction rule, which is a symmetric relation $\bowtie \subseteq B^2$;
3. a parameter $\delta$ called the delay time.

Given a bead type sequence $q \in B^*$, a conformation $c$ of $q$ is a self-avoiding path in $\mathbb{T}$ where each vertex $c_i$ is labelled by the bead type $q_i$.

We say that two bead types $a$ and $b \in B$ attract each other when $a \bowtie b$. Furthermore, given a partial conformation $c$ of a bead type sequence $q$, we say that there is a bond between two adjacent positions $c_i$ and $c_j$ of $c$ in $\mathbb{T}$ if $q_i \bowtie q_j$ and $|i - j| > 1$.

In this exercise, we shall only consider very simple Oritatami systems with delay time $\delta = 1$, in which the conformation grows one bead at a time, from a seed conformation (a few beads placed before the folding process starts, to guide the construction), and where every new bead adopts the position(s) that maximises its number of bonds with the current conformation.

Formally, given a delay-1 Oritatami system $\mathcal{O} = (p, \bowtie, 1)$ and a seed conformation $\sigma$ of a seed bead type sequence $s$, the conformation at time $0$ is $\sigma$. The conformation at time $t + 1$ is obtained by extending the conformation at time $t$ by placing the next bead, of type $p_t$, at the position(s) which maximises its number of bonds with the current conformation.

We say that the Oritatami system is deterministic if there is only one such position. We will only consider deterministic Oritatami systems in this exercise.

Example. The Oritatami system $\mathcal{O} = (p, \bowtie, 1)$ with bead types $B = \{a, b, c, d, e, f, g\}$, primary structure $p = de f g$, rule $\bowtie = \{a \bowtie g, b \bowtie d, b \bowtie e, b \bowtie f, b \bowtie g, e \bowtie g\}$ and seed conformation $\sigma = \{(0,0), a; (1,0), b; (0,-1), c\}$, folds as follows:
The seed conformation $\sigma$ is drawn in orange. The primary structure is represented by a thick black line. The bonds made are represented by dotted black lines. Note that even if $g$ is attracted by $e$, it gets placed to the west of $f$ as it makes there two bonds with $a$ and $b$.

**Shapes.** A shape is a connected subset of vertices of the triangular lattice. We want to design an Oritatami system that can fold any given shape at some suitable scale.

▶ **Question 1.1)** Exhibit a (simple) shape that cannot be folded by any given Oritatami system $\mathcal{O}$ with delay time 1. Prove it.

**Answer.** Any shape folded by an oritatami has to be Hamiltonian. Then, as the three-arms star is not Hamiltonian, it cannot be folded.

We thus need to upscale the shape if we want a general building scheme. Consider the following upsaling scheme where the vertices of the triangular lattice are replaced by non-overlapping hexagons whose sides count respectively $n + 1$, $n$, $n + 1$, $n$, $n + 1$, and $n$ vertices when considered in clockwise order starting from the north side, as shown bellow:
We say that this correspond to scale $n + 0.5$ as $n + 0.5$ is the average number of vertices per side. Note that the vertices are upscaled as unit triangles when $n = 1$. Indeed, these hexagons correspond to the consecutive concentric extensions of this unit triangle. Note that any shape is rotated by 30º counterclockwise when upscaled according to this scheme, as shown in the figure on page 6.

In the following, we will only consider scales $n + 0.5$ with $n \leq 3$.

Consider the two following paths of length 27 that cover the hexagon at scale 3.5, starting from either the smaller side (in blue), or the larger side (in black):

> **Question 1.2)** Assume that all bead types of the vertices in each path are different, identified by bead types 0, 1, \ldots, 26, and propose an attraction rule for each path that folds it with delay time $\delta = 1$ given a suitable seed conformation. Just draw the corresponding bonds on each path.

**Answer:**

> **Question 1.3)** Describe an algorithm which, given a shape $S$ of the triangular lattice as an input, outputs a path, foldable with delay time $\delta = 1$, which fills exactly an upscaled version of $S$ at scale 3.5.

**Answer:** Note that in the filling patterns below, the path-edges marked with a pink arrow can be used to extend the path to cover the neighboring cells using the filling pattern.

Indeed, the molecule can make bonds (in red) on the three pink beads (inside the green triangle just before the pink arrow) to start the new extension path from the begin of the pink arrow and get back to the end of the pink arrow to resume the current path.

We then fill each cell one after the other in some arbitrary depth-first search order starting from an arbitrary cell. Here is an example of the resulting path:
Observe that if we color every vertex \((x, y)\) of the triangular lattice with color \((2x + 3y) \mod 19\), then every of the 19 vertices at distance at most 2 from a given vertex receives a different color in \(\{0, \ldots, 18\}\), as shown in the figure below displaying the color offset modulo 19 with the gray vertex.

\[ (x, y) \]

\[ -10 \quad -9 \quad -8 \quad -6 \]
\[ 7 \quad 5 \quad 3 \quad 1 \]
\[ 12 \quad 14 \quad 16 \quad 18 \]
\[ 2 \]
\[ 15 \quad 17 \]
\[ 1 \quad 3 \quad 5 \quad 7 \]
\[ 6 \quad 8 \quad 10 \]

\[ x \]

\[ y \]

\[ \textbf{Question 1.4)} \quad \text{Propose a set of bead types } B, \text{ an attraction rule } \heartsuit, \text{ and an algorithm which given a shape } S \text{ of the triangular lattice as an input, outputs a primary structure } p \in B^* \text{ and a seed conformation } \sigma \text{ such that } p \text{ folds with delay time } 1, \text{ exactly into an upscaled version of } S \text{ at scale } 3.5. \text{ What is the size of } B? \]

\[ \text{Answer:} \quad \heartsuit \text{ Consider 19 bead types, one for each color. We say that two bead types attract each other if their corresponding colors are neighbors (as the coloring scheme is an affine function, the bonding scheme is properly defined: every color has always the same neighboring colors). We assign to each bead, the bead type corresponding to the color of its desired position. Then, every bead can only make bonds with beads of the neighboring colors of its color. Now, remark that in the bonding scheme given in answer to question } 2 \text{ the pointed bead can only be reached from the desired position, and nowhere else. It follows by induction, that the position that maximizes the number of bonds for every bead, is always the desired position. The folding is then correct.} \]

\[ \textbf{Question 1.5)} \quad \text{Show that there is a shape at scale } 1.5 \text{ which cannot be folded by any Ori-tatami system with delay time } 1. \text{ Prove it.} \]

\[ \text{Answer:} \quad \heartsuit \text{ The 3-arms star at scale } 1.5 \text{ is non-hamiltonian, and thus "non-orientatable".} \]
Question 1.6) (Optional) What about scale 2.5?

Answer. This is an open question... The 3-arms star at scale 2.5 is presumed to be non-orientamizable. Any input is welcome.
A shape $S$

The shape $S$ at scale 1.5

The shape $S$ at scale 2.5

The shape $S$ at scale 3.5

Figure 1: Example of upscaling of a shape.