HW3 Molecular Programming

M2IF CR07

2023.10.10 - Due on Fri. 10.20 before 13:30

You are asked to complete the exercise marked with a [★] and to send me your solutions to:
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as a PDF file named **HW3-Lastname.pdf** on **Fri. 10.20 before 13:30**.

■ **Exercise 1 (Oritatami).** Let first us recall the definition of an Oritatami system:

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

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

1. a bead type sequence $p \in B^*$, called the *transcript*;
2. an *attraction rule*, which is a symmetric relation $\heartsuit \subseteq B^2$;
3. a parameter δ called the *delay*.

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

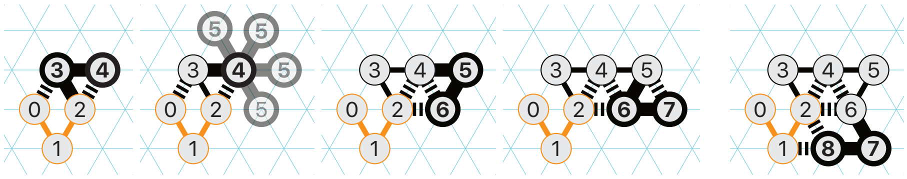
We say that two bead types a and $b \in B$ *attract* each other when $a \heartsuit b$. Furthermore, given a partial configuration c of a bead type sequence q, we say that there is a *bond* between two adjacent positions c_i and c_j of c in $\mathbb{T}$ if $q_i \heartsuit q_j$ and $|i - j| > 1$.

Notations. We denote by $c^{\rhd\delta}$ the set of all configurations extending configuration c by δ beads. We call *nascent* the δ last beads of an extension $c' \in c^{\rhd\delta}$. We denote by $h(c)$ the number of bonds made in a configuration c. We denote by $h_i(c)$ the number of bonds made with the bead indexed i in c. Given an extension $c' \in c^{\rhd\delta}$ we denote by $n(c')$ the number of bonds made by the nascent beads in c': $n(c') = h(c') - h(c)$.

Oritatami growth dynamics. Given an OS $\mathcal{O} = (p, \heartsuit, \delta)$ and a *seed configuration* σ of a *seed bead type sequence* s, the configuration at time 0 is $c^0 = \sigma$. We index negatively the beads of $\sigma = \sigma_{-|\sigma|+1} \dots \sigma_0$ so that the non-seed beads are indexed from 1 to t in configuration c^t at time t. The configuration c^{t+1} at time $t + 1$ is obtained by extending the configuration c^t at time t by placing the next bead, of type p_{t+1}, at the position(s) that maximize(s) the number of bonds over all the possible extensions of configuration c^t by δ beads. We call *favorable extension* any such extension by δ beads which maximizes the number of bonds. We denote by $F(c) = \arg\max_{\gamma \in c^{\rhd\delta}} h(\gamma)$ the set of all favorable extensions of c by δ beads. When the maximizing position is always unique (i.e. if all favorable extension always place the next bead p^{t+1} at the same location), we say that the OS is *deterministic*. We will only consider deterministic OS in this exercise.

We say that an OS is *non-blocking* if at all step, all favorable extensions can be extended by at least one bead.

Example. The OS $\mathcal{O} = (p, \heartsuit, \delta = 2)$ with bead types $\mathcal{B} = \{0, \dots, 8\}$, transcript $p = \langle 3, 4, 5, 6, 7, 8 \rangle$, rule $\heartsuit = \{0 \heartsuit 3, 0 \heartsuit 6, 1 \heartsuit 8, 2 \heartsuit 4, 2 \heartsuit 6, 2 \heartsuit 8, 4 \heartsuit 6, 5 \heartsuit 7\}$ and seed configuration $\sigma = \langle 0@(0,0); 1@(1,1); 2@(1,0) \rangle$, folds deterministically as follows:



$t = 1$ $t = 2$ $t = 3$ $t = 4$ $t = 5$

The seed configuration σ is drawn in orange. The folded transcript is represented by a black line. The bonds made are represented by dotted black lines. The $\delta = 2$ nascent beads are represented in bold. If there are several favorable extensions, the freely moving nascent part is represented translucently. Observe two remarkable steps:

- $t = 2$ and 3: the position of 5 is not determined when 4 is placed (indeed, there are several favorable extensions placing 5 at different locations), but will be fixed when 5 and 6 are folded together.
- $t = 4$ and 5: 7 is initially placed next to 5 when 6 and 7 are folded together but will be finally placed to the right of 8 when 7 and 8 are folded together (because two bonds can be made there instead of only one) and 7 will thus remain there.

Crucial step. Consider a deterministic OS. Let us denote by c^∞ its final configuration. We say that step t is *crucial* for the nascent bead indexed by k if all favorable extensions of c^{t-1} agree to place bead indexed by k at its final location in c^∞ whereas it was not the case for all the favorable extensions of c^{t-2}. For instance, there are exactly two crucial steps in the example above: steps 3 and 5 which are crucial for beads 5 and 7 respectively.

We now consider a non-blocking deterministic OS.

▶ Question 1.1) *Prove that for all configuration $c' \in c^{t \triangleright \delta}$, $n(c') \leqslant 4\delta + 1$.*

▷ *Hint. how many bonds can make a nascent bead?*

Answer. ▷ Every bead in the molecule has two neighbors in the primary structure except for the last who has only one. Each bead has thus at most 4 (5 for the last bead) potential neighbors to bond with. The maximum number of nascent bonds is thus: $4(\delta - 1) + 5$. ◁

▶ Question 1.2) *Prove that: if for some $1 \leqslant i < \delta$, there is $c' \in F(c^{t-1})$ such that c' and c^∞ disagree on the position of the bead indexed by $t + i$ (i.e., $c'_{t+i} \neq c^\infty_{t+i}$), then there is a crucial step t' with $t < t' < t + \delta$.*

Answer. ▷ If some nascent bead is misplaced at some step t, it has to be placed correctly before it become non-nascent, which occurs on or before step $t + \delta - 1$, thus there is a crucial step among step $t + 1, \dots, t + \delta - 1$. ◁

Let us denote by $N(c)$ the maximum number of bonds made by nascent beads in an extension of c: $N(c) = \max_{\gamma \in c^{\triangleright \delta}} n(\gamma) = \max_{\gamma \in c^{\triangleright \delta}} h(\gamma) - h(c)$.

▶ Question 1.3) *Prove that at all time t, for a non-blocking OS:*

1. $N(c^{t-1}) \leqslant N(c^t) + h_t(c^t)$
2. *furthermore, if step t is crucial, then:* $N(c^{t-1}) \leqslant N(c^t) + h_t(c^t) - 1$

Answer. ▷ Consider a δ-elongation $c' \in F(c^{t-1})$. As the OS is deterministic, c' and c^t agree on the position of the bead indexed by t that becomes non-nascent at time t. As the OS is non-blocking, c' can be extended by one bead into a configuration c'' which is thus a δ-elongation c'' of c^t (as c^t and c' agree on the position of the bead indexed t). By definition, $n(c'') \leqslant N(c^t)$ and $n(c') = N(c^{t-1})$. And, the number of nascent bonds in c''

verifies: $n(c'') \geqslant n(c') - h_t(c^t)$ as bead indexed by t is non-nascent in c'' but non-nascent in c' and as the righthand ignores the bonds of the last nascent bead in c''. It follows that: $N(c^t) \geqslant N(c^{t-1}) - h_t(c^t)$ (1). Now, observe that if step t is crucial for some bead k, then choose above for c' a favorable δ-elongation that misplace bead k, c'' must not be favorable which means that $N(c^t) > n(c'')$, which yields (2). $\triangleleft$

We want to prove that there is no non-blocking OS that can fold a long enough straight line. By contradiction, let's consider a deterministic OS $\mathcal{O}$ with delay δ and a seed σ whose terminal configuration is a straight line of length L.

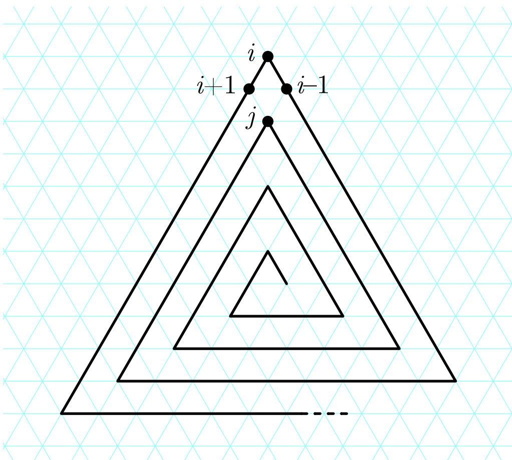
▶ **Question 1.4)** *Show that at all step t, there is always a favorable extension of c^{t-1} that does not place the last nascent bead, indexed by $t + \delta - 1$, at its final position.*
Answer. $\triangleright$ c^∞ been a straight line, c^t is always a prefix of this straight line. It follows that the only elongation that places the last nascent bead at the correct location is a straight line too. Note that rotating the segment made of the δ nascent bead yields an elongation with the same number of bonds, so if there is one favorable elongation which places correctly the last nascent bead, there are others which don't, so it is never stabilized in its final position. $\triangleleft$

▶ **Question 1.5)** *Show that there are at least $\lfloor (L - |\sigma|)/\delta \rfloor$ crucial steps in the folding of $\mathcal{O}$.*
Answer. $\triangleright$ Let's partition time into disjoint time-segment of length δ: $\{k\delta, \ldots, k(\delta + 1) - 1\}$ for $0 \leqslant k < L/\delta$. According to question 1.4, the last bead is not stabilized at every time $k\delta$, thus, by question 1.2, there is a crucial step in $\{k\delta + 1, \ldots, k(\delta + 1) - 1\}$. There are thus at least $\lfloor (L - |\sigma|)/\delta \rfloor$ crucial steps. $\triangleleft$

▶ **Question 1.6)** *Conclude that $L \leqslant |\sigma| + O(\delta^2)$.*
Answer. $\triangleright$ Note that as c^t is a straight line, $h_t(c^t) = 0$ for all t. It follows by question 1.3 that $N(c^t)$ is non-decreasing and increases at every crucial time steps: $N(c^t) \geqslant N(c^{t-1})$ and $N(c^t) \geqslant N(c^{t-1}) + 1$ if step t is crucial. As there are at least $\lfloor (L - |\sigma|)/\delta \rfloor$ crucial steps, $N(c^\infty) \geqslant (L - |\sigma|)/\delta - 1$. But as $N(c^t) \leqslant 4\delta + 1$ for all t by question 1.1, we have: $L - \sigma \leqslant 4\delta^2 + 2\delta$ which concludes the proof. $\triangleleft$

It follows that there is no non-blocking deterministic OS that can fold into a long enough straight line. Surprisingly enough, there is a blocking deterministic delay-6 OS that can fold into arbitrary long straight line!

[★] Exercise 2 (Oritatami — Impossible triangle path). We want to prove that no deterministic oritatami system with delay $\delta \leqslant 2$ can fold according to the infinite triangular spiral below. Recall that the transcript t of an oritatami system (t is the sequence of bead types) is *ultimately periodic*, i.e. there is an i_0 and a period T such that for all $i \geqslant 0$, $t_{i_0+i} = t_{i_0+T+i}$.

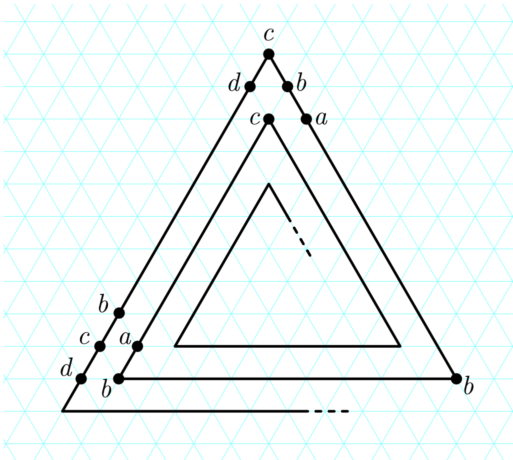


► **Question 2.1)** *Prove than no deterministic delay-1 oritatami system can fold according to this spiral.*
Answer. ▷ The bead at the corner cannot make any bond with anyone, it is thus impossible to place correctly at delay 1. ◁

Let us consider now a deterministic delay-2 oritatami system that would fold according to the infinite triangular spiral.

► **Question 2.2)** *Prove that 2 bonds are required to place the bead correctly at each corner.*
Answer. ▷ Using the notations at the top corner from the figure, let i be the index of the bead at a corner. At delay 2, only i and $i+1$ can make bonds. i cannot make bonds with anyone from its final position. If i is placed correctly, $i+1$ can only make bonds with j and $i-1$. In all case, if $i+1$ makes only one bond, the triangle $(i-1)i(i+1)$ can move around and i is not stabilized. Thus, 2 bonds are needed and 2 bonds are enough: $(i+1)$—$(i-1)$ and $(i+1)$—j. ◁

► **Question 2.3)** *Show that there are 4 consecutive bead types a, b, c, d in the transcript that get placed as follows:*



Answer. ▷ Consider i_0 be the index from which the transcript is periodic and let $T > i_0$ be a multiple of its period larger than i_0. Consider the side of length T in the spiral and let b be the identical bead type at its two extremities and let a, c and d be the preceding and the two following bead types respectively. They are located as illustrated above. ◁

► **Question 2.4)** *Show that in order to stabilize c in the lower left corner, c must bind with a.*
Answer. ▷ From question 2.2, in order to fold the top corner properly, d must bind with b. Thus, in the lower left corner, when folding c and d, d can make two bonds with the two bs if located at c's place. At least three bonds must then be made in order to place c at its correct location. Furthermore, only three bonds can be made if c is at its correct location: d—b, c—a and c—b. It follows that c must bind to a. ◁

► **Question 2.5)** *Conclude that c cannot be placed deterministically at the top corner.*
Answer. ▷ When c and d are folded at the top corner, only two bonds can be made if c is correctly located. But, if c and d are located to the east and to the north-east of b resp., c binds with a and d with b. c is thus unstable and cannot be placed correctly deterministically. ◁

► **Question 2.6 (★★★))** *What about deterministic oritatami systems with larger delays?*
Answer. ▷ We suspect it is impossible for all delay, but... no one never knows until it's proven... help wanted! ◁