

Counting infinitely by Oritatami co-transcriptional folding

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Abstract. abstract

1 Introduction

2 Preliminaries

Let Σ be a finite set of types of abstract molecules, or *beads*. A bead of type $a \in \Sigma$ is called an a -bead. By Σ^* and Σ^ω , we denote the set of finite sequences of beads and that of one-way infinite sequences of beads, respectively. The empty sequence is denoted by λ . Let $w = b_1b_2 \cdots b_n \in \Sigma^*$ be a sequence of length n for some integer n and bead types $b_1, \dots, b_n \in \Sigma$. The *length* of w is denoted by $|w|$, that is, $|w| = n$. For two indices i, j with $1 \leq i \leq j \leq n$, we let $w[i..j]$ refer to the subsequence $b_ib_{i+1} \cdots b_{j-1}b_j$; if $i = j$, then $w[i..i]$ is simplified as $w[i]$. For $k \geq 1$, $w[1..k]$ is called a *prefix* of w .

Oritatami systems fold their transcript, which is a sequence of beads, over the triangular grid graph $\mathbb{T} = (V, E)$ cotranscriptionally. We designate one point in V as the origin O of \mathbb{T} . For a point $p \in V$, let \odot_p^d denote the set of points which lie in the regular hexagon of radius d centered at the point p . Note that \odot_p^d consists of $3d(d+1) + 1$ points. A directed path $P = p_1p_2 \cdots p_n$ in \mathbb{T} is a sequence of *pairwise-distinct* points $p_1, p_2, \dots, p_n \in V$ such that $\{p_i, p_{i+1}\} \in E$ for all $1 \leq i < n$. Its i -th point is referred to as $P[i]$. Now we are ready to abstract RNA single-stranded structures in the name of conformation. A *conformation* C (over Σ) is a triple (P, w, H) of a directed path P in \mathbb{T} , $w \in \Sigma^*$ of the same length as P , and a set of h-interactions $H \subseteq \{\{i, j\} \mid 1 \leq i, i+2 \leq j, \{P[i], P[j]\} \in E\}$. This is to be interpreted as the sequence w being folded along the path P in such a manner that its i -th bead $w[i]$ is placed at the i -th point $P[i]$ and the i -th and j -th beads are bound (by a hydrogen-bond-based interaction) if and only if $\{i, j\} \in H$. The condition $i+2 \leq j$ represents the topological restriction that two consecutive beads along the path cannot be bound. The *length* of C is defined to be the length of its transcript w (that is, equal to the length of the path P). A *rule set* $R \subseteq \Sigma \times \Sigma$ is a symmetric relation over Σ , that is, for all bead types $a, b \in \Sigma$, $(a, b) \in R$ implies $(b, a) \in R$. A bond $\{i, j\} \in H$ is *valid*

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with respect to R , or simply R -valid, if $(w[i], w[j]) \in R$. This conformation C is R -valid if all of its bonds are R -valid. For an integer $\alpha \geq 1$, C is of *arity* α if it contains a bead that forms α bonds but none of its beads forms more. By $C_{\leq \alpha}(\Sigma)$, we denote the set of all conformations over Σ whose arity is at most α ; its argument Σ is omitted whenever Σ is clear from the context.

The oritatami system grows conformations by an operation called elongation. Given a rule set R and an R -valid conformation $C_1 = (P, w, H)$, we say that another conformation C_2 is an elongation of C_1 by a bead $b \in \Sigma$, written as $C_1 \xrightarrow{R}_b C_2$, if $C_2 = (Pp, wb, H \cup H')$ for some point $p \in V$ not along the path P and set $H' \subseteq \{\{i, |w| + 1\} \mid 1 \leq i < |w|, \{P[i], p\} \in E, (w[i], b) \in R\}$ of bonds formed by the b -bead; this set H' can be empty. Note that C_2 is also R -valid. This operation is recursively extended to the elongation by a finite sequence of beads as: for any conformation C , $C \xrightarrow{R}_\lambda^* C$; and for a finite sequence of beads $w \in \Sigma^*$ and a bead $b \in \Sigma$, a conformation C_1 is elongated to a conformation C_2 by wb , written as $C_1 \xrightarrow{R}_{wb}^* C_2$, if there is a conformation C' that satisfies $C_1 \xrightarrow{R}_w^* C'$ and $C' \xrightarrow{R}_b C_2$.

An *oritatami system* (OS) $\Xi = (\Sigma, R, \delta, \alpha, \sigma, w)$ is composed of

- a set Σ of bead types,
- a rule set $R \subseteq \Sigma \times \Sigma$,
- a positive integer δ called the *delay*,
- a positive integer α called the *arity*,
- an initial R -valid conformation $\sigma \in C_{\leq \alpha}(\Sigma)$ called the *seed*, whose first bead is assumed to be at the origin O without loss of generality,
- a (possibly infinite) *transcript* $w \in \Sigma^* \cup \Sigma^\omega$, which is to be folded upon the seed 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 bonds a conformation has, the more stable it gets. The set $\mathcal{F}(\Xi)$ of conformations *foldable* by the system Ξ 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

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

Then we say that the bead $w[i+1]$ and the bonds it forms are *stabilized* according to C_{i+1} . The easiest way to understand this stabilization process should be the video available at <https://www.dailymotion.com/video/x3cdj35>, in which the Turing universal oritatami system by Geary et al. [1], whose delay is 3, is running. 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 .

References

1. Geary, C., Meunier, P.E., Schabanel, N., Seki, S.: Proving the Turing universality of oritatami cotranscriptional folding. In: Proc. ISAAC 2018 (2018), in press