Iterated Hairpin Completions of Non-crossing Words

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DNA Strand

Sequence of nukleobases
Adenine, Cytosine, Guanine, Thymine

$5'$−C−G−G−T−A−T−C−A−T−C−C−C−A−$3'$

DNA Biochemistry

DNA Strand

Sequence of nukleobases
Adenine, Cytosine, Guanine, Thymine

Watson-Crick complement

$\overline{\mathsf{A}} = \mathsf{T}$ and $\overline{\mathsf{C}} = \mathsf{G}$

$$5'-C-G-G-T-A-T-C-A-T-C-C-C-A-3'$$
$$3'-G-C-C-A-T-A-G-T-A-G-G-G-T-5'$$

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$$\begin{array}{c} 5'-\text{C}-\text{G}-\text{G}-\text{T}-\text{A}-\text{T}-\text{C}-\text{A}-\text{T}-\text{C}-\text{C}-\text{C}-\text{A}-3' \\ 3'-\text{G}-\text{C}-\text{C}-\text{A}-\text{T}-\text{A}-\text{G}-\text{T}-\text{A}-\text{G}-\text{G}-\text{G}-\text{T}-5' \end{array}$$

Formal Languages

Alphabet Σ
Complement $\overline{} : \Sigma \to \Sigma$
$\overline{a_1 \cdots a_m} = \overline{a_m} \cdots \overline{a_1}$

Polymerase Chain Reaction (PCR)

Template $\tau = \sigma\alpha$

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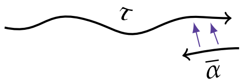

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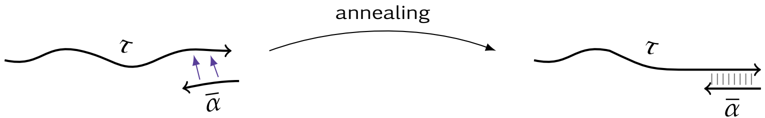

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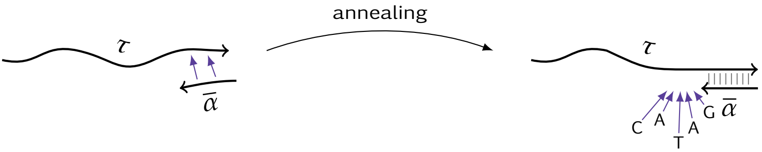

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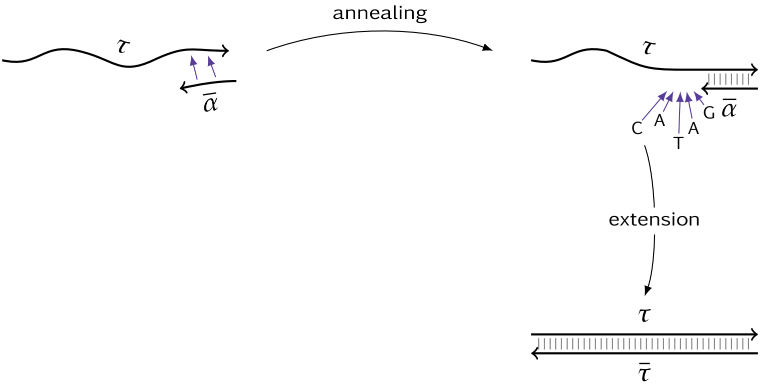

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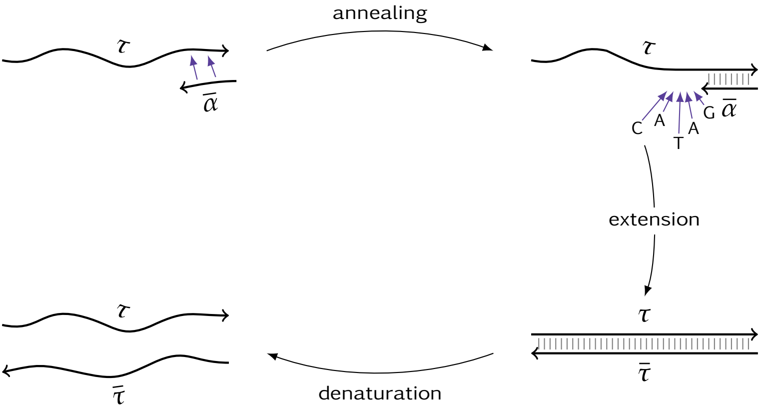

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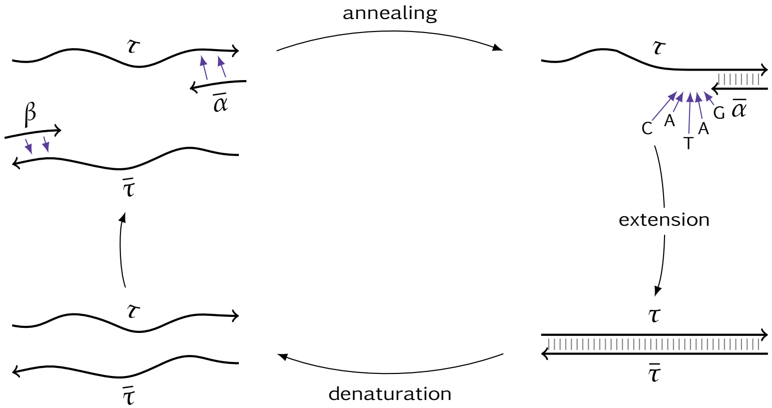

Template $\tau = \sigma\alpha = \beta\sigma'$

Primer $\bar{\alpha}, \beta$

Hairpin Completion

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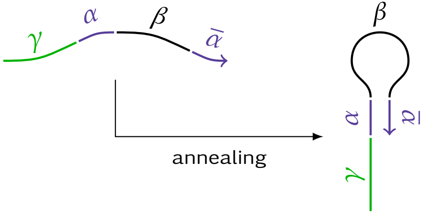

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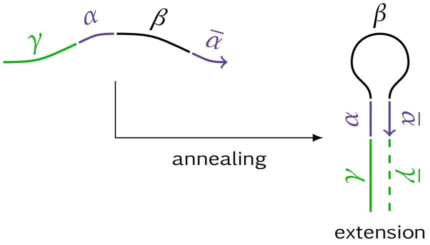

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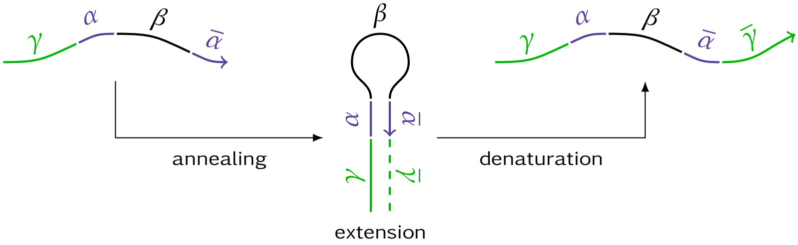

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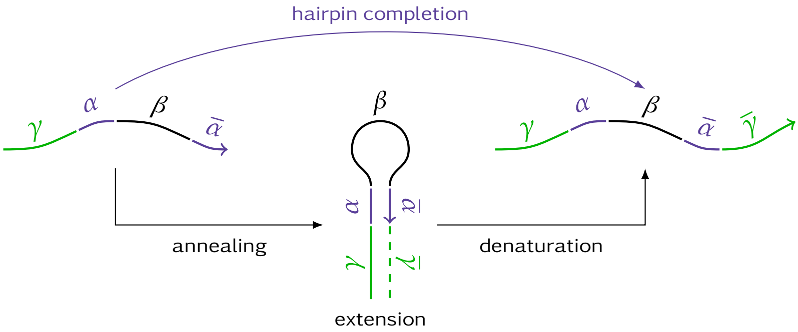

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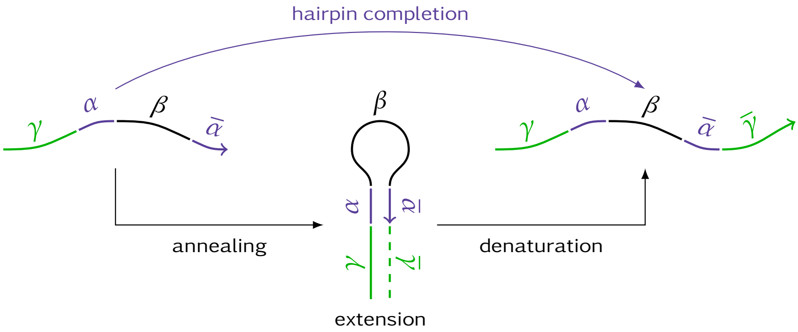

Primer: α

Hairpin completion:

$$\gamma\alpha\beta\overline{\alpha} \to_{\mathcal{R}} \gamma\alpha\beta\overline{\alpha}\overline{\gamma} \qquad \alpha\beta\overline{\alpha}\overline{\gamma} \to_{\mathcal{L}} \gamma\alpha\beta\overline{\alpha}\overline{\gamma}$$

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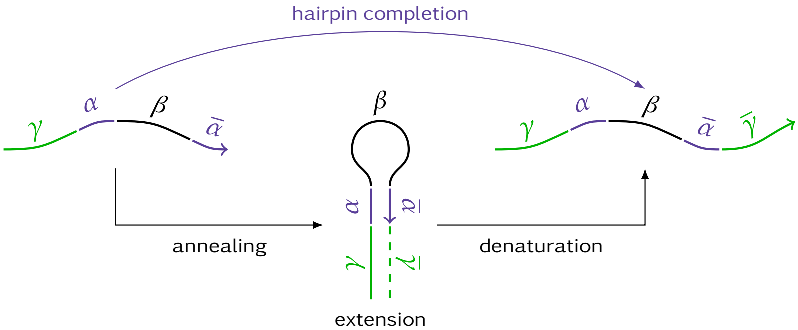

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$$w \rightarrow z \qquad \text{if } w \rightarrow_{\mathcal{R}} z \text{ or } w \rightarrow_{\mathcal{L}} z$$

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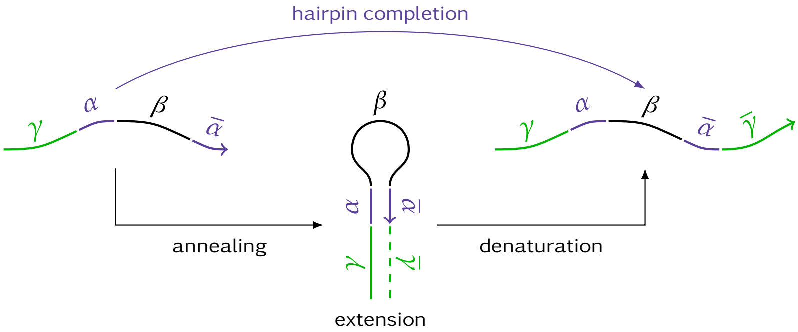

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$$w \rightarrow z \qquad \text{if } w \rightarrow_{\mathcal{R}} z \text{ or } w \rightarrow_{\mathcal{L}} z$$

Iterated hairpin completion:

$$\mathcal{H}^*(w) = \{z \mid w \rightarrow^* z\}$$

Example

$$\alpha b \alpha c \alpha \overline{\alpha} \bar{d} \overline{\alpha} \bar{d} \overline{\alpha}$$

Example

$$\underline{\alpha b}\alpha c\alpha\overline{\alpha}\overline{d}\overline{\alpha}\overline{d}\overline{\alpha}\overline{b}\overline{\alpha}$$

Example

$$\underline{\alpha b}\alpha c \alpha \overline{\alpha}\bar{d}\overline{\alpha}\bar{d}\overline{\alpha}(\bar{b}\overline{\alpha})^i$$

Example

$$\underline{\alpha b \alpha c}\,\alpha\overline{\alpha}\bar{d}\overline{\alpha}\bar{d}\overline{\alpha}(\bar{b}\overline{\alpha})^{i}\bar{c}\overline{\alpha}\bar{b}\overline{\alpha}$$

Example

$$abac(ab)^i ad abaca\bar{a}\bar{d}\bar{a}\bar{d}\bar{a}(\bar{b}\bar{a})^i\bar{c}\bar{a}\bar{b}\bar{a}$$

Example

$$\alpha b \alpha c (\alpha b)^i \alpha d \alpha b \alpha c (\alpha b)^i \alpha d \alpha b \alpha c \alpha \overline{\alpha} \bar{d} \overline{\alpha} \bar{d} \overline{\alpha} (\bar{b} \overline{\alpha})^i \bar{c} \overline{\alpha} \bar{b} \overline{\alpha}$$

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$$\alpha b\alpha c(\alpha b)^i\alpha d\alpha b\alpha c(\alpha b)^i\alpha d\underbrace{\alpha b\alpha c\alpha\overline{\alpha}\bar{d}\overline{\alpha}\bar{d}\overline{\alpha}}_{=z}(\bar{b}\overline{\alpha})^i\bar{c}\overline{\alpha}\bar{b}\overline{\alpha}$$

Proposition

$\mathcal{H}^*(z)$ is not context-free.

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Proposition

$\mathcal{H}^*(z)$ is not context-free.

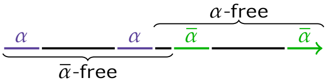
Questions

i.) Is $\mathcal{H}^*(w) \overset{?}{\in} \mathrm{REG}$ decidable?

ii.) Does $w \in \Sigma^*$ exist such that $\mathcal{H}^*(w)$ is context-free but not regular?

Non-crossing Words

w is non-crossing $\iff$



e. g., $z = \alpha b \alpha c \alpha \overline{\alpha} \bar{d} \overline{\alpha} \bar{d} \overline{\alpha}$ is non-crossing

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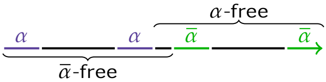

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Every word in $\mathcal{H}^*(w)$ is non-crossing if w is non-crossing.

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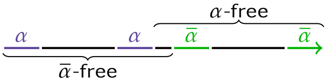

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Theorem (main result)

For non-crossing $w \in \Sigma^*$

i.) $\mathcal{H}^*(w) \overset{?}{\in} \mathrm{REG}$ *is decidable.*

ii.) $\mathcal{H}^*(w)$ *is either regular or not context-free.*

Non-regularity of $\mathcal{H}^*(z)$

Let w be non-crossing.
$P_\alpha(w) = \{p_0, \ldots, p_m\}$ s. t. $p_i\alpha$ is a prefix of w.

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If $m, n \geq 1$, then $\mathcal{H}^*(w) = \{w\} \cup \bigcup_{1 \leq i \leq m} \mathcal{H}^*(w\overline{p_i}) \cup \bigcup_{1 \leq i \leq n} \mathcal{H}^*(s_i w)$.

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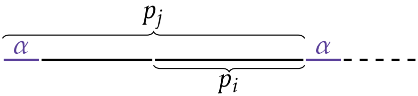

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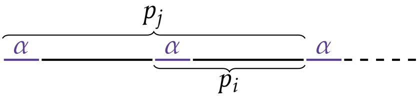

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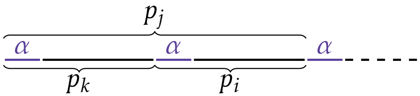

$\Rightarrow p_j = p_k p_i$

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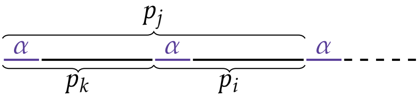

$\Rightarrow p_j = p_k p_i$ $\Rightarrow w\overline{p_i} \rightarrow_{\mathcal{R}} w\overline{p_i}\,\overline{p_k} = w\overline{p_j}$ $\Rightarrow w\overline{p_j} \in \mathcal{H}^*(w\overline{p_i})$

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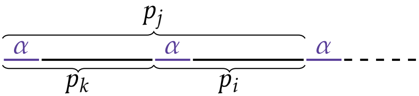

$\Rightarrow p_j = p_k p_i$ $\Rightarrow w\overline{p_i} \to_{\mathcal{R}} w\overline{p_i}\overline{p_k} = w\overline{p_j}$ $\Rightarrow w\overline{p_j} \in \mathcal{H}^*(w\overline{p_i})$

Lemma

Let $P = \{p_1, \ldots, p_m\} \setminus \{p_1, \ldots, p_m\}^2$, $S = \{s_1, \ldots, s_m\} \setminus \{s_1, \ldots, s_m\}^2$, and $p_1 \neq s_1$.

- $\mathcal{H}^*(w) = \{w\} \cup \bigcup_{p \in P} \mathcal{H}^*(w\bar{p}) \cup \bigcup_{s \in S} \mathcal{H}^*(sw)$ *and the union is disjoint.*

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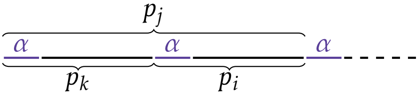

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- *$\mathcal{H}^*(w) = \{w\} \cup \bigcup_{p \in P} \mathcal{H}^*(w\bar{p}) \cup \bigcup_{s \in S} \mathcal{H}^*(sw)$ and the union is disjoint.*
- *$\mathcal{H}^*(w)$ is regular iff $\forall p \in P$: $\mathcal{H}^*(w\bar{p})$ is regular and $\forall \bar{s} \in S$: $\mathcal{H}^*(sw)$ is regular.*

Non-regularity of $\mathcal{H}^*(z)$

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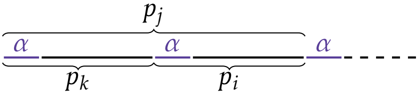

$\Rightarrow p_j = p_k p_i$ $\quad\Rightarrow w\overline{p_i} \rightarrow_{\mathcal{R}} w\overline{p_i}\overline{p_k} = w\overline{p_j}$ $\quad\Rightarrow w\overline{p_j} \in \mathcal{H}^*(w\overline{p_i})$

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- $\mathcal{H}^*(w) = \{w\} \cup \bigcup_{p \in P} \mathcal{H}^*(w\bar{p}) \cup \bigcup_{s \in S} \mathcal{H}^*(sw)$ *and the union is disjoint.*
- $\mathcal{H}^*(w)$ *is regular iff* $\forall p \in P$: $\mathcal{H}^*(w\bar{p})$ *is regular and* $\forall \bar{s} \in S$: $\mathcal{H}^*(sw)$ *is regular.*

Example

$z = \alpha b \alpha c \alpha \bar{\alpha}\bar{d}\bar{\alpha}\bar{d}\bar{\alpha}$:
$\mathcal{H}^*(z) = \{z\} \cup \mathcal{H}^*(z\bar{b}\bar{\alpha}) \cup \mathcal{H}^*(z\bar{c}\bar{\alpha}\bar{b}\bar{\alpha}) \cup \mathcal{H}^*(\alpha d z) \cup \mathcal{H}^*(\alpha d \alpha d z)$

Non-regularity of $\mathcal{H}^*(z)$

Theorem

Assume $p_1 = s_1$. $\mathcal{H}^*(w)$ *is regular iff*

1. $p_i \in \overline{S_{\overline{\alpha}}(w)}^*$ *or* $\overline{S_{\overline{\alpha}}(w)} \subseteq \{p_1, \ldots, p_i\}^*$ *for all* $i \leq m$ *and*
2. $s_i \in P_\alpha(w)^*$ *or* $P_\alpha(w) \subseteq \{s_1, \ldots, s_i\}^*$ *for all* $i \leq n$.

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$z = \alpha b \alpha c \alpha \overline{\alpha} \bar{d} \overline{\alpha} \bar{d} \overline{\alpha}$:
$\mathcal{H}^*(z)$ is regular iff $\mathcal{H}^*(z\bar{b}\overline{\alpha})$, $\mathcal{H}^*(z\bar{c}\overline{\alpha}\bar{b}\overline{\alpha})$, and $\mathcal{H}^*(\alpha d z)$ are regular.

1. $P_\alpha(\alpha d z) = \{\varepsilon, \alpha d, \alpha d \alpha b, \alpha d \alpha b \alpha c\}$ $\quad \overline{S_{\overline{\alpha}}(\alpha d z)} = \{\varepsilon, \alpha d, \alpha d \alpha d\}$

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1. $P_\alpha(\alpha d z) = \{\varepsilon, \alpha d, \alpha d \alpha b, \alpha d \alpha b \alpha c\}$ $\overline{S_{\overline{\alpha}}(\alpha d z)} = \{\varepsilon, \alpha d, \alpha d \alpha d\}$
   $\Rightarrow \mathcal{H}^*(\alpha d z)$ is regular. $\mathcal{H}^*(\alpha d z)$ is regular.

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Example

$z = \alpha b \alpha c \alpha \overline{\alpha} \bar{d} \overline{\alpha} \bar{d} \overline{\alpha}$:
$\mathcal{H}^*(z)$ is regular iff $\mathcal{H}^*(z\bar{b}\overline{\alpha})$, $\mathcal{H}^*(z\bar{c}\overline{\alpha}\bar{b}\overline{\alpha})$, and $\mathcal{H}^*(\alpha d z)$ are regular.

1. $P_\alpha(\alpha d z) = \{\varepsilon, \alpha d, \alpha d \alpha b, \alpha d \alpha b \alpha c\}$ $\qquad \overline{S_{\overline{\alpha}}(\alpha d z)} = \{\varepsilon, \alpha d, \alpha d \alpha d\}$
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2. $P_\alpha(z\bar{b}\overline{\alpha}) = \{\varepsilon, \alpha b, \alpha b \alpha c\}$ $\qquad \overline{S_{\overline{\alpha}}(z\bar{b}\overline{\alpha})} = \{\varepsilon, \alpha b, \alpha b \alpha d, \alpha b \alpha d \alpha d\}$

Non-regularity of $\mathcal{H}^*(z)$

Theorem

Assume $p_1 = s_1$. $\mathcal{H}^*(w)$ is regular iff

1. $p_i \in \overline{S_{\overline{\alpha}}(w)}^*$ *or* $\overline{S_{\overline{\alpha}}(w)} \subseteq \{p_1, \ldots, p_i\}^*$ *for all* $i \leq m$ *and*
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Questions?

Thank you!