

Iterated Hairpin Completions of Non-crossing Words

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DNA Biochemistry

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

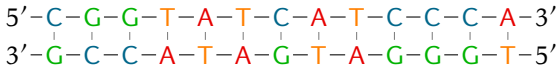
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Watson-Crick complement

$\bar{A} = T$ and $\bar{C} = G$



DNA Biochemistry

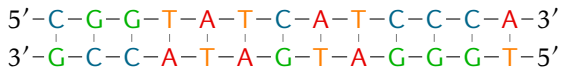
DNA Strand

Sequence of nukleobases

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Formal Languages

Alphabet Σ

Complement $\bar{\cdot} : \Sigma \rightarrow \Sigma$

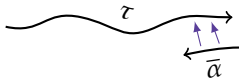
$$\overline{a_1 \cdots a_m} = \bar{a}_m \cdots \bar{a}_1$$

Polymerase Chain Reaction (PCR)



Template $\tau = \sigma\alpha$

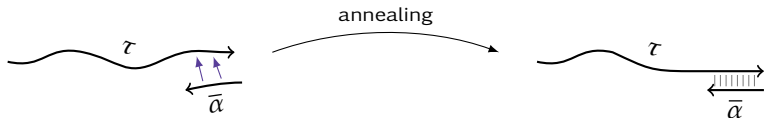
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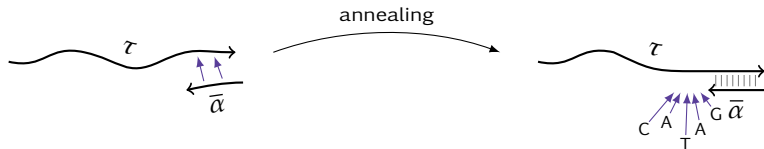
Primer $\bar{\alpha}$

Polymerase Chain Reaction (PCR)



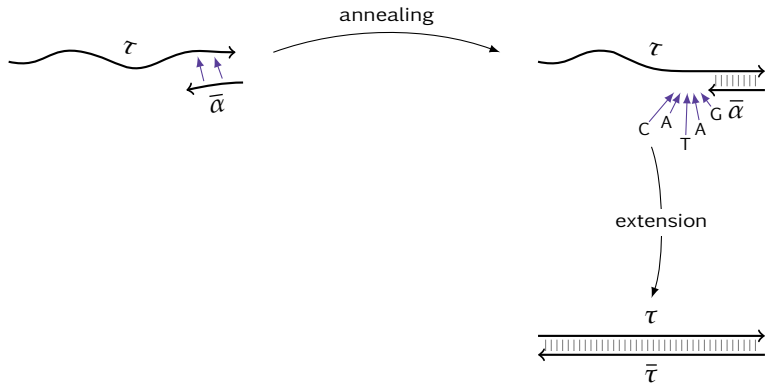
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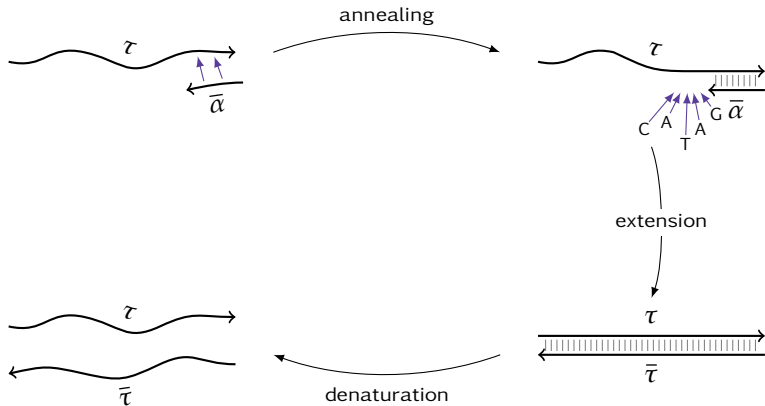
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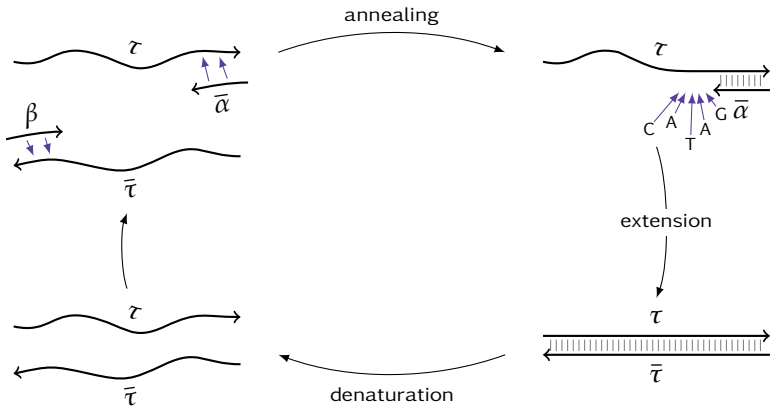
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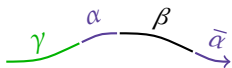
Template $\tau = \sigma\alpha$
 Primer $\bar{\alpha}$

Polymerase Chain Reaction (PCR)

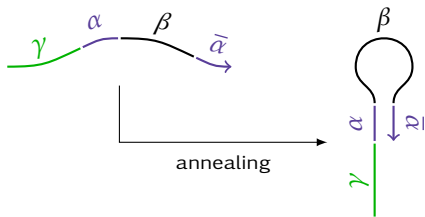


Template $\tau = \sigma\alpha = \beta\sigma'$
 Primer $\bar{\alpha}, \beta$

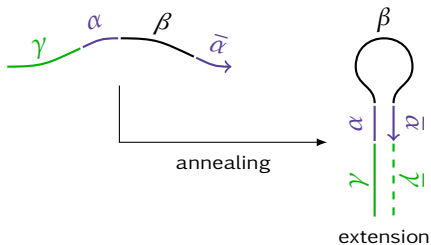
Hairpin Completion



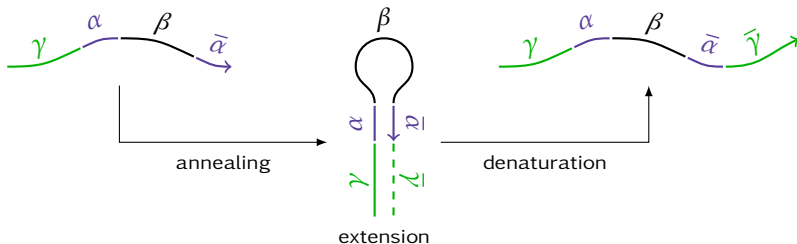
Hairpin Completion



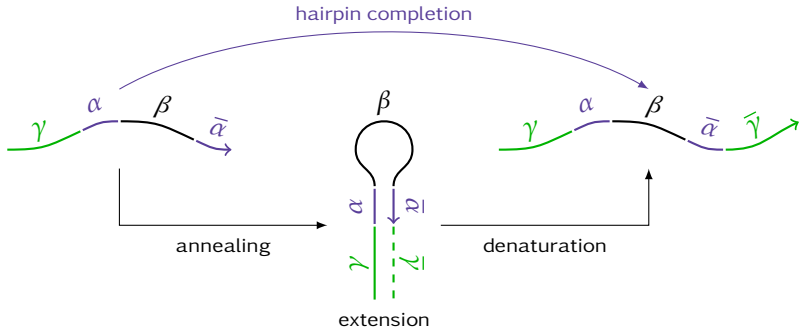
Hairpin Completion



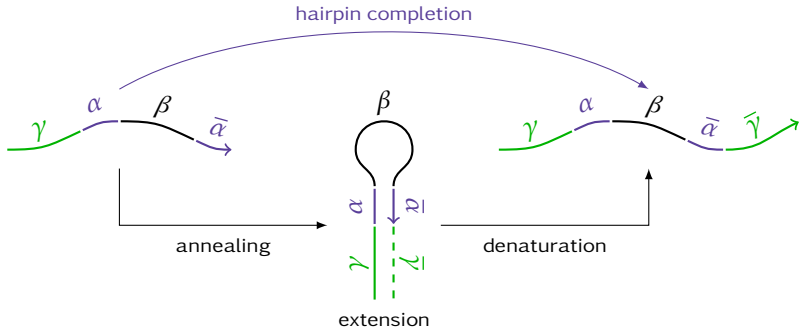
Hairpin Completion



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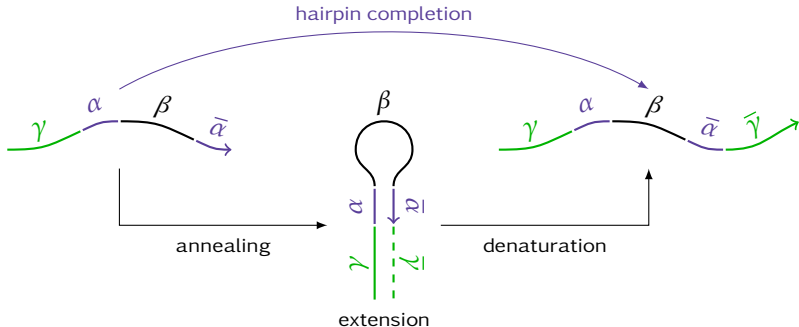
Primer: α

Hairpin completion:

$$\gamma\alpha\beta\bar{\alpha} \rightarrow_{\mathcal{R}} \gamma\alpha\beta\bar{\alpha}\bar{\gamma}$$

$$\alpha\beta\bar{\alpha}\bar{\gamma} \rightarrow_{\mathcal{L}} \gamma\alpha\beta\bar{\alpha}\bar{\gamma}$$

Hairpin Completion



Primer: α

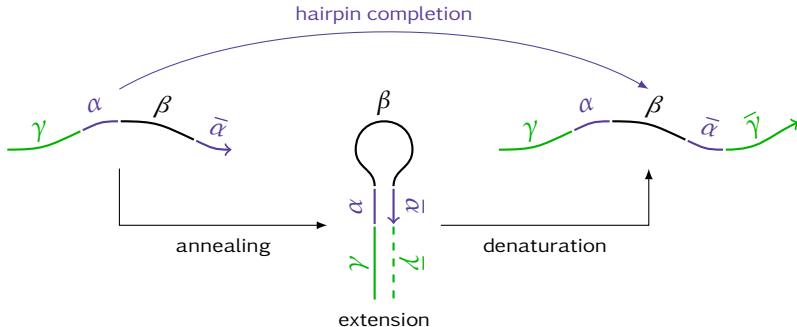
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$$w \rightarrow z \quad \text{if } w \rightarrow_{\mathcal{R}} z \text{ or } w \rightarrow_{\mathcal{L}} z$$

Hairpin Completion



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Iterated hairpin completion:


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

Example

$ab\alpha c\alpha\bar{\alpha}\bar{d}\bar{\alpha}\bar{d}\bar{\alpha}$


Example

$ab\alpha c\alpha\bar{a}\bar{d}\bar{a}\bar{d}\bar{a}\bar{b}\bar{a}$




Example

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

A diagram showing a word with a bracket under the first part and an arrow pointing to the end of the word. The word is $ab\alpha c\alpha\bar{\alpha}d\bar{\alpha}d\bar{\alpha}(\bar{b}\bar{\alpha})^i$. A horizontal line is drawn under the first part of the word, starting from the 'a' and ending under the 'd' of the first $\bar{\alpha}$. From the right end of this line, a curved arrow points upwards and then to the right, ending at the end of the word.

Example


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



The diagram shows the word $\alpha b \alpha c \alpha \bar{\alpha} \bar{d} \bar{\alpha} \bar{d} \bar{\alpha} (\bar{b} \bar{\alpha})^i \bar{c} \bar{\alpha} \bar{b} \bar{\alpha}$. A horizontal purple line is drawn under the first four characters $\alpha b \alpha c$. A purple arrow starts from the right end of this line and points to the right, ending under the character \bar{c} in the sequence $(\bar{b} \bar{\alpha})^i \bar{c} \bar{\alpha} \bar{b} \bar{\alpha}$.


Example

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



Example

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Example

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Example

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

Proposition

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

Example

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

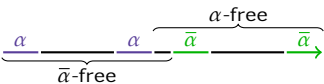
Proposition

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

Questions

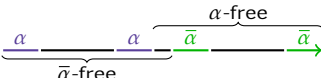
- i.) Is $\mathcal{H}^*(w) \stackrel{?}{\in} \text{REG}$ decidable?
- ii.) Does $w \in \Sigma^*$ exist such that $\mathcal{H}^*(w)$ is context-free but not regular?

Non-crossing Words

w is non-crossing \iff 

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

Non-crossing Words

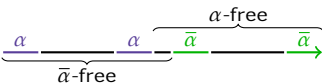
w is non-crossing \iff The diagram shows a sequence of characters on a horizontal line. From left to right: a purple α , a purple α , a green $\bar{\alpha}$, and a green $\bar{\alpha}$. A bracket below the first two α 's is labeled $\bar{\alpha}$ -free. A bracket above the last two $\bar{\alpha}$'s is labeled α -free. The final $\bar{\alpha}$ has a right-pointing arrow.

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

Proposition

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

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

Theorem (main result)

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

- i.) $\mathcal{H}^*(w) \stackrel{?}{\in} \text{REG}$ is decidable.
- ii.) $\mathcal{H}^*(w)$ is either regular or not context-free.

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

Let w be non-crossing.

$P_\alpha(w) = \{p_0, \dots, p_m\}$ s. t. $p_i\alpha$ is a prefix of w .

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Example

$z = \alpha b \alpha c \alpha \bar{\alpha} \bar{d} \bar{\alpha} \bar{d} \bar{\alpha}$:

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

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Lemma

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

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Example

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

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

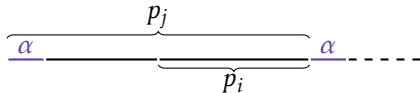
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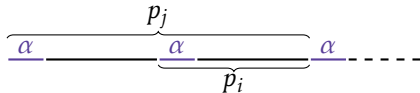
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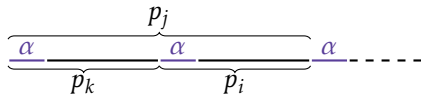
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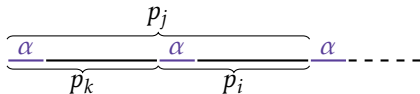


$$\Rightarrow p_j = p_k p_i$$

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

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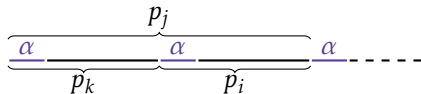
$$\Rightarrow w\bar{p}_i \rightarrow_{\mathcal{R}} w\bar{p}_i \bar{p}_k = w\bar{p}_j$$

$$\Rightarrow w\bar{p}_j \in \mathcal{H}^*(w\bar{p}_i)$$

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

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Lemma

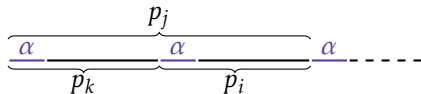
Let $P = \{p_1, \dots, p_m\} \setminus \{p_1, \dots, p_m\}^2$, $S = \{s_1, \dots, s_m\} \setminus \{s_1, \dots, s_m\}^2$, and $p_1 \neq s_1$.

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

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

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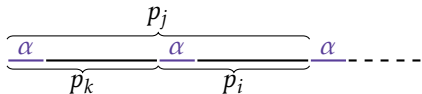
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- ▶ $\mathcal{H}^*(w)$ is regular iff $\forall p \in P: \mathcal{H}^*(w\bar{p})$ is regular and $\forall \bar{s} \in S: \mathcal{H}^*(s\bar{s})$ is regular.

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

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If p_i is a suffix of p_j , then $\mathcal{H}^*(w\bar{p}_j) \subseteq \mathcal{H}^*(w\bar{p}_i)$.



$$\Rightarrow p_j = p_k p_i$$

$$\Rightarrow w\bar{p}_i \rightarrow_{\mathcal{R}} w\bar{p}_i \bar{p}_k = w\bar{p}_j$$

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- ▶ $\mathcal{H}^*(w)$ is regular iff $\forall p \in P: \mathcal{H}^*(w\bar{p})$ is regular and $\forall s \in S: \mathcal{H}^*(sw)$ is regular.

Example

$$z = \alpha b \alpha c \alpha \bar{a} \bar{d} \bar{a} \bar{d} \bar{a}:$$

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

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

Theorem

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

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

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Example

$z = \alpha b \alpha c \alpha \bar{\alpha} \bar{d} \bar{\alpha} \bar{d} \bar{\alpha}$:

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

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 $\Rightarrow \mathcal{H}^*(\alpha dz)$ is regular. $\mathcal{H}^*(\alpha dz)$ is regular.

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$z = ab\alpha c\alpha\bar{\alpha}\bar{d}\bar{\alpha}\bar{d}\bar{\alpha}$:

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

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

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

Theorem

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

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

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Questions?

Thank you!