On Hairpin-Free Words and Languages

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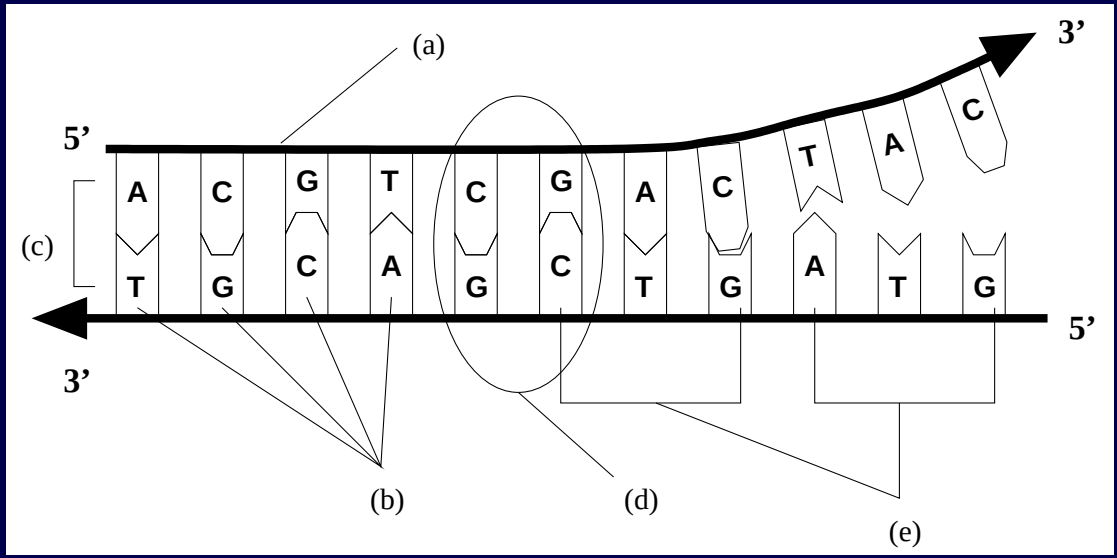
A DNA molecule



A segment of a double-stranded DNA molecule. (a) Sugar-phosphate backbone, with a 5' $\rightarrow$ 3' orientation; (b) nucleotides; (c) bindings; (d) Watson-Crick complementarity principle; (e) triples of nucleotides: *codons.*

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- The DNA complementarity involution γ is a morphism given by $\gamma(A) = T$, $\gamma(T) = A$, $\gamma(C) = G$, $\gamma(G) = C$.
- Example: $\epsilon(ACGCTG) = ACGCTG = \mu(GTCGCA) = \gamma(TGCGAC)$.

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- Example: $\epsilon(ACGCTG) = ACGCTG = \mu(GTCGCA) = \gamma(TGCGAC)$.
- The Watson-Crick involution $\tau = \mu\gamma$ corresponds to the DNA bond formation.

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- Hairpins are the main tool used in the Whiplash PCR computing techniques.
- Hairpins serve as a binary information medium for DNA RAM.
- Hairpins are a basic component of "smart drugs."

Formalization of hairpins

Definition 1 *Let θ be a morphic or antimorphic involution of X^*, let $k \geq 1$, then a word $u \in X^*$ is said to be θ-k-hairpin-free or simply hp(θ,k)-free if $u = xvy\theta(v)z$ for some $x, v, y, z \in X^*$ implies $|v| < k$.*

Observe: if $v = 1$, the empty word, $\theta = \epsilon$, the identity involution, and $k = 1$, then a word u is hp(ϵ,1)-free iff it is square-free.

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Definition 3 *A language L is called θ-k-hairpin-free or simply hp(θ, k)-free if $L \subseteq hpf(\theta, k)$.*

Observe: L is hp(θ, k)-free *iff* $X^*vX^*\theta(v)X^* \cap L = \emptyset$ for all $|v| \geq k$.

Examples

1. Let $X = \{a, b\}$ with $\theta(a) = b, \theta(b) = a$. Then:

$$hpf(\theta, 1) = a^* \cup b^*$$

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3. Let $\theta = \mu$ be the mirror involution and let $X = \{a, b\}$, then:

$$hpf(\theta, 1) = \{1, a, b, ab, ba\}$$

Observe: if $\theta = \mu$, then $hpf(\theta, 1)$ is always finite.

Properties of hp$(\theta, 1)$-free languages

Definition 4 *(i) A language L is* $\leq_e$-convex *if $u \leq_e w \leq_e v$, $u, v \in L$ implies $w \in L$.* *(ii) L is* right $\leq_e$-convex *if $u \leq_e w$, $u \in L$ implies $w \in L$.*

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Definition 6 *Let H be a nonempty subset of X^+.*

(i) We denote $S(H) = \{w \in X^* | u \leq_e w, u \in H\}$.

(ii) H is called a hypercode over X^* iff *$x \leq_e y$ and $x, y \in H$ imply $x = y$.*

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Proposition 7 *Let θ be an involution. Then there exists a unique hypercode H such that $hp(\theta, 1) = S(H)$.*

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Proposition 10 *Consider a binary alphabet* X. *Then* $hpf(\mu, k)$ *is finite if and only if* $k \leq 4$.

Proposition 11 *Let* θ *be an involution. The language* $hpf(\theta, k)$ *over a non-singleton alphabet* X *is finite if and only if one of the following holds:*
(a) $\theta = \epsilon$, *the identity involution;*
(b) $\theta = \mu$, *the mirror involution, and either* $k = 1$ *or* $|X| = 2$ *and* $k \leq 4$.

Decidability of hp(θ, k)-freedom

Corollary 12 *The following problem is decidable in linear time w.r.t.* $|M|$*:*

Input: *An NFA* M*.*

Output: *Yes/No depending on whether* $L(M)$ *is* $hp(\theta, k)$*-free.*

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Corollary 13 *The following problem is decidable in linear time w.r.t.* $|M_1| \cdot |M_2|$*:*

Input: *A DFA* M_1 *such that* $L(M_1)$ *is* $hp(\theta, k)$*-free, and a NFA* M_2*.*

Output: *Yes/No depending on whether there is a word* $w \in L(M_2) - L(M_1)$ *such that* $L(M_1) \cup \{w\}$ *is* $hp(\theta, k)$*-free.*

The context-free case

Corollary 14 *The following problem is decidable in cubic time w.r.t.* $|M|$*:*

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Descriptional complexity issues

Proposition 16 *The number of states of a minimal NFA accepting the language* $hp(\theta, k)$, $k \geq 1$, *over an alphabet* X *of the cardinality* $\ell > 1$, *is between* ℓ^k *and* $3\ell^k$, *its size is at most* $3(\ell^k + \ell^{k+1})$.

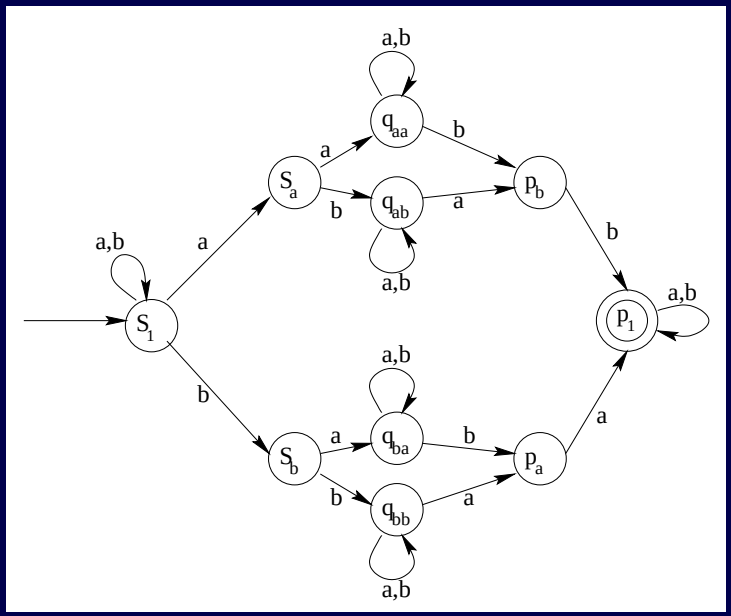

Figure 1: An example of an NFA accepting the language $hp(\theta, 2)$.

Proposition 17 *Assume that there are distinct letters* $a, b \in X$ *such that* $a = \theta(b)$. *Then the number of states of a minimal NFA accepting* $hpf(\theta, k)$, $k \geq 1$, *over an alphabet* X *with the cardinality* ℓ, *is at least* $2^{(\ell-2)^k/2}$.

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Proposition 17 *Assume that there are distinct letters $a, b \in X$ such that $a = \theta(b)$. Then the number of states of a minimal NFA accepting $hpf(\theta, k)$, $k \geq 1$, over an alphabet X with the cardinality ℓ, is at least $2^{(\ell-2)^k/2}$.*

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Corollary 19 *Consider the DNA alphabet $\Delta = \{A, C, T, G\}$ and the Watson-Crick involution τ.*

(i) The size of a minimal NFA accepting $hp(\tau, k)$ is at most $15 \cdot 4^k$. The number of its states is between 4^k and $3 \cdot 4^k$.

(ii) The number of states of either a minimal DFA or an NFA accepting $hpf(\tau, k)$ is between $2^{2^{k-1}}$ and $2^{3 \cdot 2^{2k}}$.

Thank you!