Deduplication on Finite Automata and Nested Duplication Systems

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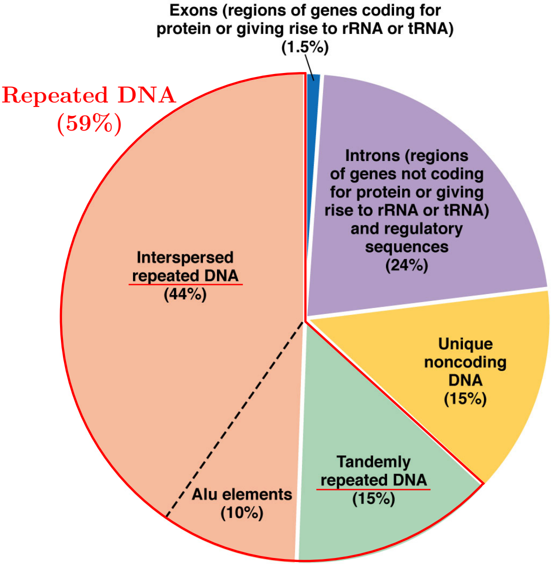
Outline

Repeated DNA in Human Genome

Human genome contains large amount of repeated DNA.



Researches on Duplications

In formal language theory, a DNA is a string over $\Sigma = \{A, G, C, T\}$.

- Duplication operation on strings and their properties
  - Searls, *"The computational linguistics of biological sequences"*, 1993.
  - Dassow et al., *"On the regularity of duplication closure"*, 1999.
  - Dassow et al., *"Operations and language generating devices suggested by the genome evolution"*, 2002.
  - Leupold et al., *"Formal languages arising from gene repeated duplication"*, 2003.
  - Leupold et al., *"Uniformly bounded duplication languages"*, 2005.
  - Ito et al., *"Duplication in DNA sequences"*, 2008.
  - Cho et al., *"Duplications and pseudo-duplications"*, 2016.
- Duplication Grammar
  - Martìn-Vide and Păun, *"Duplication grammars"*, 1999.
  - Mitrana and Rozenberg, *"Some properties of duplication grammars"*, 1999.

From Information Theory Viewpoint

Jain et al.[1] and Farnoud et al.[2] considered the string duplication systems and computed the capacity of the systems:

- *string duplication system* $S = (\Sigma, s, \tau)$ generates all strings by applying duplication function of τ to an initial string s a finite number times,
- *capacity* of string duplication system represents how many strings of length n that the system produces out of $|\Sigma^n|$, where n goes to infinity.

[1] S. Jain, F. Farnoud, and J. Bruck. *Capacity and expressiveness of genomic tandem duplication*, ISIT 2015

[2] F. Farnoud, M. Schwartz, and J. Bruck. *The capacity of string-duplication systems*, IEEE Transactions on Information Theory, 2016

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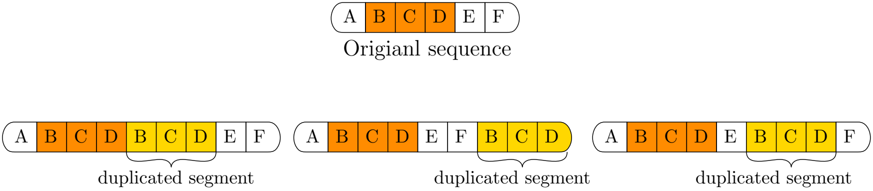

(a) Tandem duplication (b) End duplication (c) Interspersed duplication

From Information Theory Viewpoint

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- *string duplication system* generates all strings by applying duplication function to an initial string an infinity number times,
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$$cap(S) = \lim_{n \to \infty} \sup \frac{\log_{|\Sigma|} |S \cap \Sigma^n|}{n}$$

From Information Theory Viewpoint

The *Capacity* of string duplication system represents how many strings of length n the system produces out of $|\Sigma^n|$, where n goes to infinity.

Example

From a string 01 over $\Sigma = \{0, 1\}$, a system duplicates any substring of length up to 2 from 01 repetitively.

- $01 \rightarrow 011 \rightarrow 01111 \rightarrow 0101111...$

Then, the number of strings of length n is 2^{n-2}.

Encoding strings of length n in this system need $n-2$ bits.

The average number of bits per symbol = 1

From Information Theory Viewpoint

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Then, the number of strings of length n is 2^{n-2}.

Encoding strings of length n in this system need $n-2$ bits.

The capacity of this system = 1

From Information Theory Viewpoint

For computing the capacity, $\lim_{n\to\infty} \sup \frac{\log_{|\Sigma|} |S \cap \Sigma^n|}{n}$, of the duplication system $S = (\Sigma, s, \tau)$, we need to consider all strings

- of length n, where n goes to infinity,
- iteratively obtained by a duplication function $\mathbb{D} \in \tau$ from an initial string s,

$$\mathbb{D}^i(\mathbb{D}^{i-1}(\cdots(\mathbb{D}^2(\mathbb{D}^1(s))))), \text{ for } i \geq 1.$$

Jain et al. (2015)

Given a finite directed graph that represents the string duplication system S, we can compute the capacity of S using *Perron-Frobenus Theory* [Lind and Marcus, 1985].

It is hard to construct a finite automata!

Our Goal from Formal Language Theory

1. Define a variant of duplication functions named *nested tandem duplication*
2. Construct an NFA for a set of strings obtained by a nested duplication system
   - NFA construction (possible for any restriction on length of duplicated substring)
   - $\mathbb{D}$-cycle deduplication on NFA
3. Compute the capacity of the nested duplication system

Definition of Nested Duplication

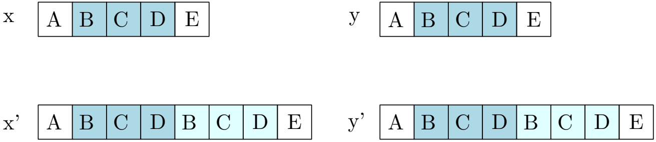
Definition (Tandem Duplication)

A tandem duplication $\mathbb{D}^{tan}_{\leq k}$ of x is defined

$$\mathbb{D}^{tan}_{\leq k}(x) = \begin{cases} uvvw & \text{for } x = uvw, |u| = i, |v| \leq k \\ x & \text{otherwise.} \end{cases}$$

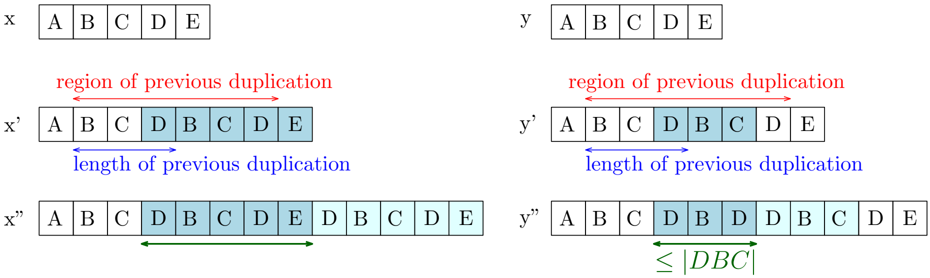
For a string x, $\mathbb{D}^{tan}_{\leq k}(x)$ allows a substring v of length up to k starting at position $i+1$ to be duplicated next to its original position.

Tandem Duplication and Nested Duplication



(a) A tandem duplication (b) A nested duplication

Tandem Duplication and Nested Duplication



(a) A tandem duplication

(b) A nested duplication

Definition of Nested Duplication

Definition (Nested Duplication)

A nested duplication $\mathbb{D}^{nes}_{\leq k}$ of x with a array d is defined $\mathbb{D}^{nes}_{\leq k}(x, d)$=

$$\begin{cases} (uvvw, d[1 : |u|] \cdot |v|^{2|v|} \cdot d[|u|+|v|+1 : |x|]) & \text{if } d[j] \geq |v| \\ & \text{for } |u|+1 \leq j \leq |u|+|v|, \\ (x, d) & \text{otherwise.} \end{cases}$$

- For a string $w = w_1 w_2 \cdots w_n$ and $i \geq 1$, $w[1 : i]$ denotes a substring $w_1 \cdots w_i$.
- For an integer $j \geq 1$, j^k denotes k consecutive j.

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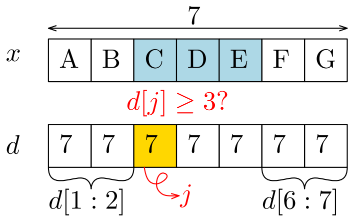

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$$(y, d') \in \mathbb{D}^{nes}_{2,3}(x, d)$$

y	A	B	C	D	E	C	D	E	F	G
d'	7	7	3	3	3	3	3	3	7	7

$d[1:2]$ $\quad$ 3^{3*2} $\quad$ $d[2+3+1:7]$

Definition of Nested Duplication

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y	A	B	C	D	E	C	D	E	F	G
d'	7	7	3	3	3	3	3	3	7	7

$d'[j] \geq 4?$

j

Definition of Nested Duplication

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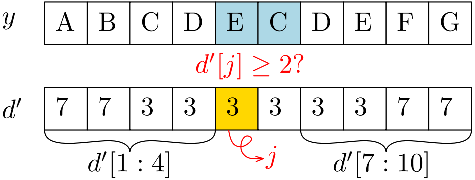

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$$(z, d'') \in \mathbb{D}^{nes}_{\leq 3}(z, d'')$$

z	A	B	C	D	E	C	E	C	D	E	F	G
d''	7	7	3	3	2	2	2	2	3	3	7	7

$d'[1:4]$ 2^{2*2} $d'[7:10]$

Nested Duplication System

Definition (Nested Duplication System)

A *nested duplication system* consists of three tuples $S = (\Sigma, s, \mathbb{D}^{nes}_{\leq k})$,

- $s \in \Sigma^*$ is seed, a finite length string,
- $\mathbb{D}^{nes}_{\leq k}$ is the nested duplication function.

We call the set of all strings generated by the system $S = (\Sigma, s, \mathbb{D}^{nes}_{\leq k})$

the language generated by S, $L(S)$.

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We extend the nested duplication system to a language

$$S = (\Sigma, L, \mathbb{D}^{nes}_{\leq k}).$$

NFA Construction for $L(S)$

We construct an NFA M_S recognizing the language $L(S)$ generated by the nested duplication system $S = (\Sigma, s, \mathbb{D}^{nes}_{\leq k})$.

NFA Construction for $L(S)$

An NFA M_S is a tuple $(Q, \Sigma, \delta, 0_0, \{n_0\})$, where

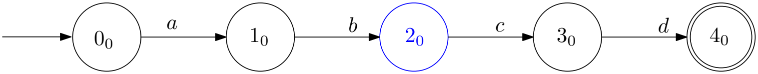
$$Q = \{q \mid q = l[1]_{d[1]} l[2]_{d[2]} \cdots l[t]_{d[t]}, 1 \leq t \leq n, d[1] = 0\}$$

- t represents the depth of a duplication, $1 \leq t \leq n$
- for each depth t, $d[t]$ denotes the length of duplications,
- $l[t]$ represents $\#$ of characters duplicated so far by the last duplication in depth t.

NFA Construction for $L(S)$

$S = (\Sigma, abcd, \mathbb{D}^{nes}_{\leq 4})$

$q = l[1]_{d[1]} l[2]_{d[2]} \cdots l[t]_{d[t]}$



$\delta((i-1)_0, s[i]) = i_0$

- duplication depth$= 0$
- two characters are so far read

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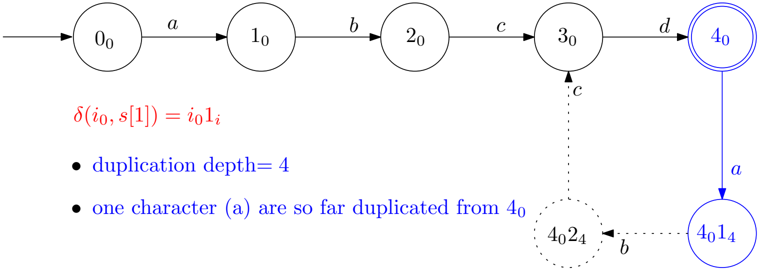

$\delta(i_0, s[1]) = i_0 1_i$

- duplication depth= 4
- one character (a) are so far duplicated from 4_0

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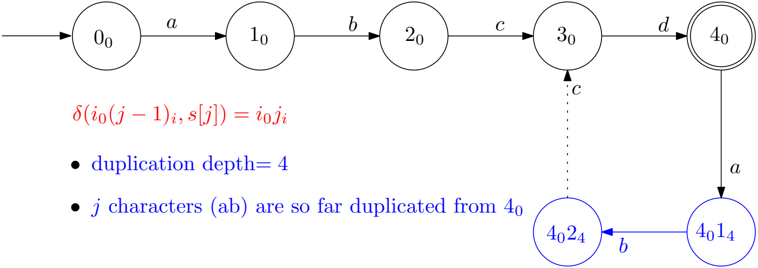

$\delta(i_0(j-1)_i, s[j]) = i_0 j_i$

- duplication depth $= 4$
- j characters (ab) are so far duplicated from 4_0

NFA Construction for $L(S)$

$S = (\Sigma, abcd, \mathbb{D}^{nes}_{\leq 4})$

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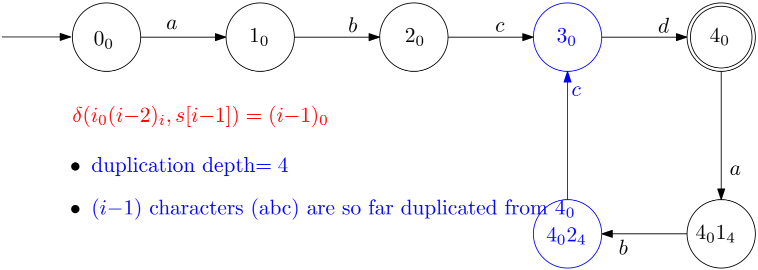


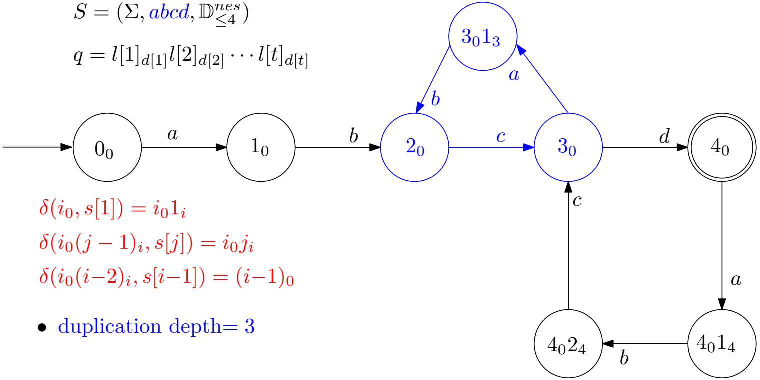
$\delta(i_0(i-2)_i, s[i-1]) = (i-1)_0$

- duplication depth= 4
- $(i-1)$ characters (abc) are so far duplicated from 4_0

NFA Construction for $L(S)$

$S = (\Sigma, abcd, \mathbb{D}^{nes}_{\leq 4})$

$q = l[1]_{d[1]} l[2]_{d[2]} \cdots l[t]_{d[t]}$



$\delta(i_0, s[1]) = i_0 1_i$

$\delta(i_0 (j-1)_i, s[j]) = i_0 j_i$

$\delta(i_0 (i-2)_i, s[i-1]) = (i-1)_0$

- duplication depth= 3

NFA Construction for $L(S)$

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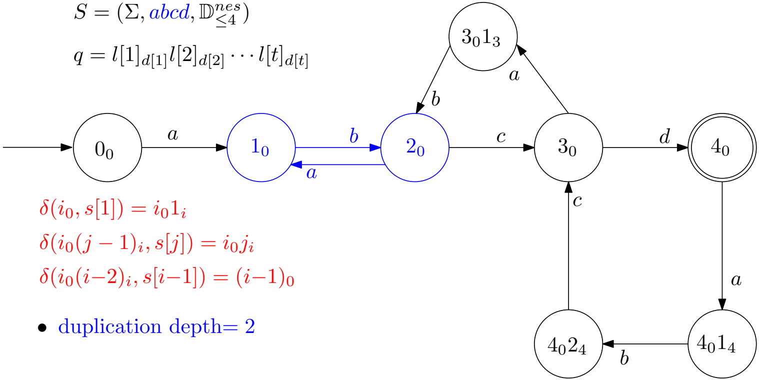


$\delta(i_0, s[1]) = i_0 1_i$

$\delta(i_0 (j-1)_i, s[j]) = i_0 j_i$

$\delta(i_0 (i{-}2)_i, s[i{-}1]) = (i{-}1)_0$

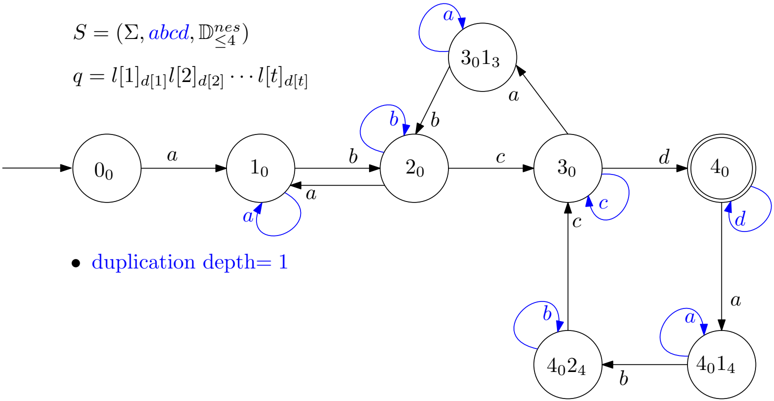
- duplication depth= 2

NFA Construction for $L(S)$

$S = (\Sigma, abcd, \mathbb{D}^{nes}_{\leq 4})$

$q = l[1]_{d[1]} l[2]_{d[2]} \cdots l[t]_{d[t]}$

- duplication depth$= 1$



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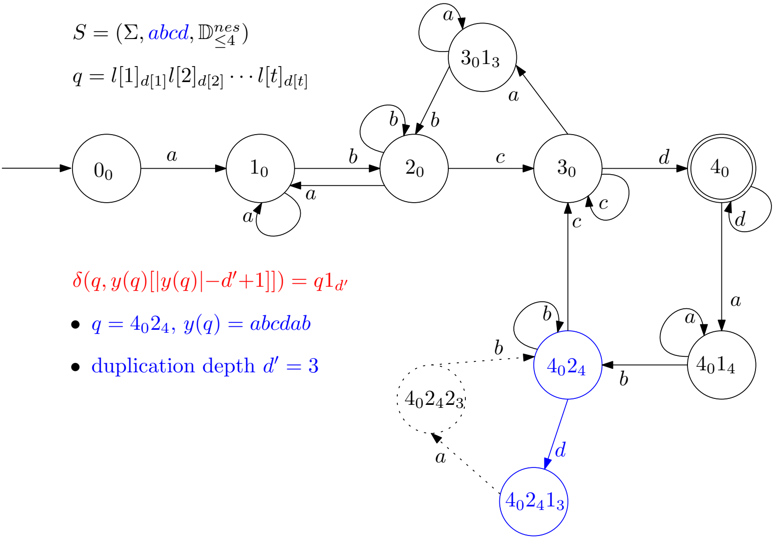

$\delta(q, y(q)[|y(q)| - d' + 1]) = q1_{d'}$

- $q = 4_0 2_4,\ y(q) = abcdab$
- duplication depth $d' = 3$

NFA Construction for $L(S)$

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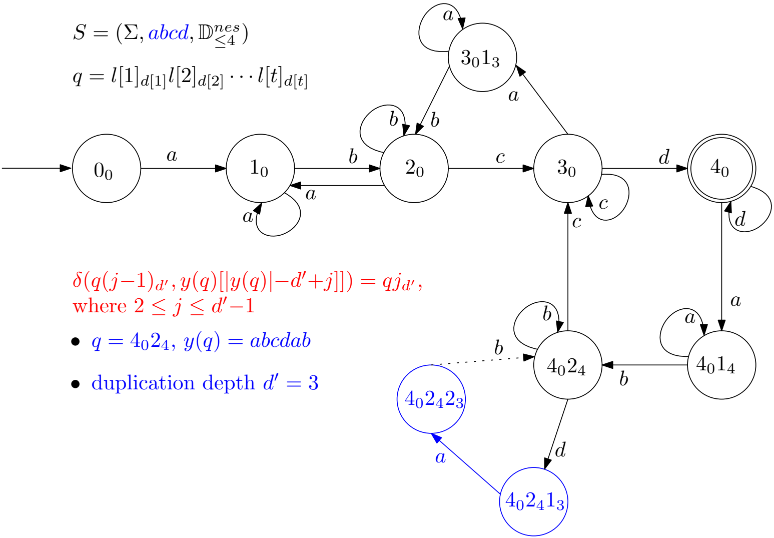
$q = l[1]_{d[1]} l[2]_{d[2]} \cdots l[t]_{d[t]}$



$\delta(q(j-1)_{d'}, y(q)[|y(q)|-d'+j]) = qj_{d'}$,
where $2 \leq j \leq d'-1$

- $q = 4_0 2_4$, $y(q) = abcdab$
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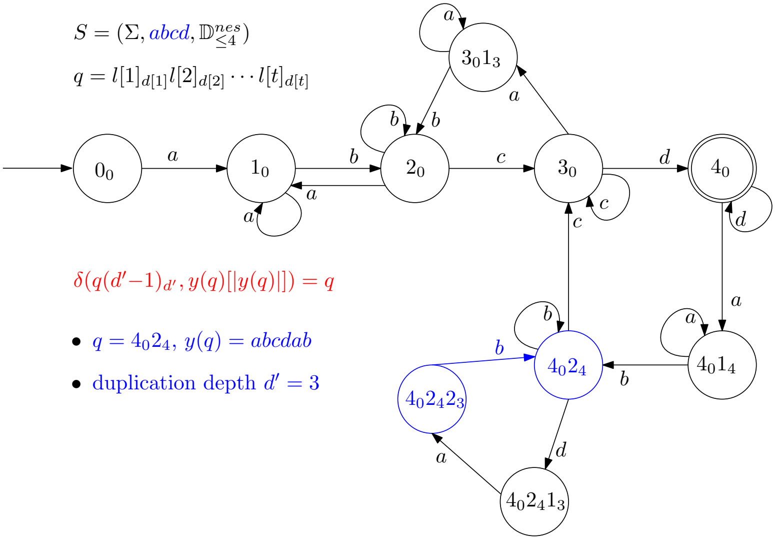

$\delta(q(d'-1)_{d'}, y(q)[|y(q)|]) = q$

- $q = 4_0 2_4$, $y(q) = abcdab$
- duplication depth $d' = 3$

NFA Construction for $L(S)$

$S = (\Sigma, abcd, \mathbb{D}^{nes}_{\leq 4})$

$q = l[1]_{d[1]} l[2]_{d[2]} \cdots l[t]_{d[t]}$

$\delta(q, y(q)[|y(q)| - d' + 1]]) = q1_{d'}$

$\delta(q(j-1)_{d'}, y(q)[|y(q)| - d' + j]]) = qj_{d'}$, where $2 \leq j \leq d' - 1$

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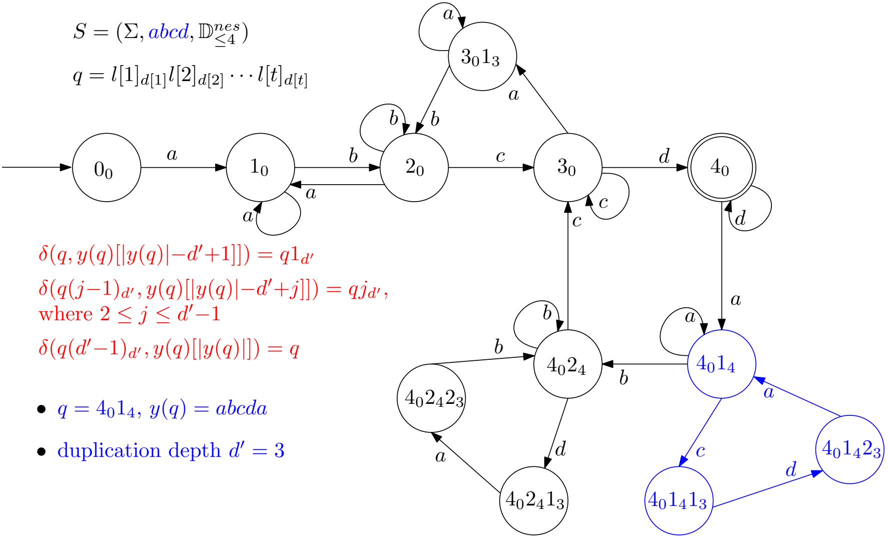

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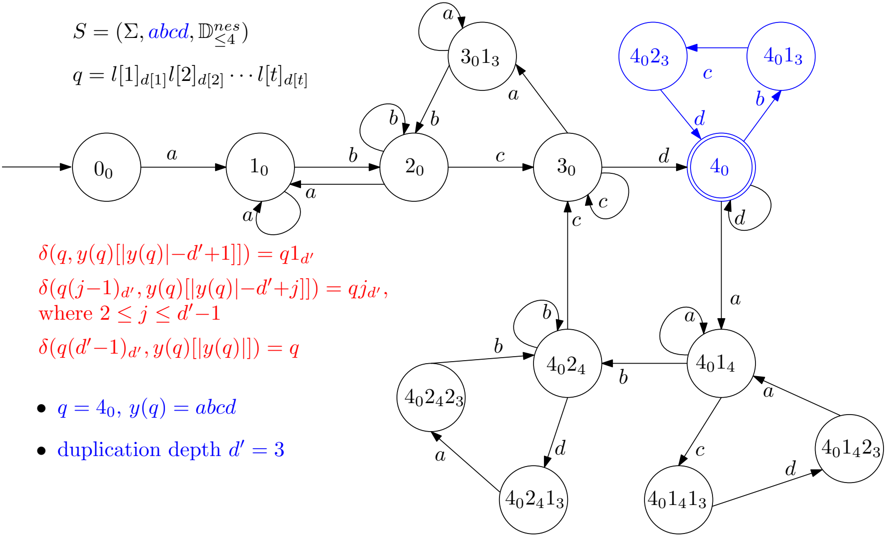
where $2 \leq j \leq d' - 1$

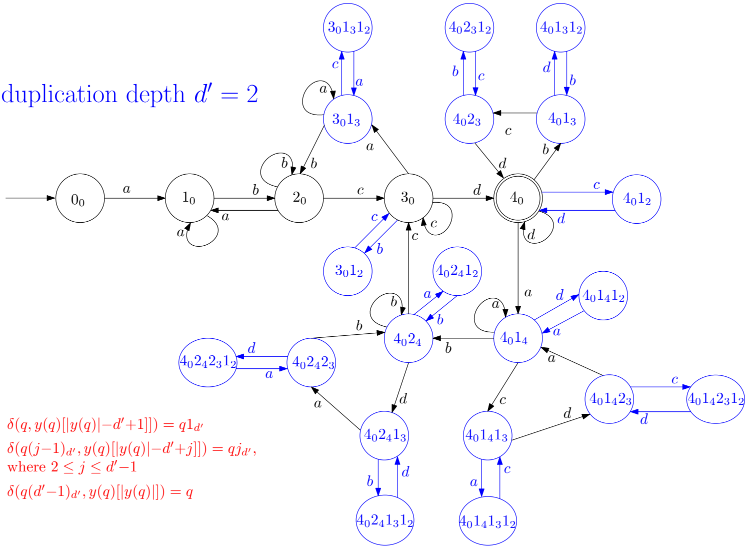
$\delta(q(d'-1)_{d'}, y(q)[|y(q)|]) = q$

- $q = 4_0$, $y(q) = abcd$
- duplication depth $d' = 3$



NFA Construction for $L(S)$

duplication depth $d' = 2$



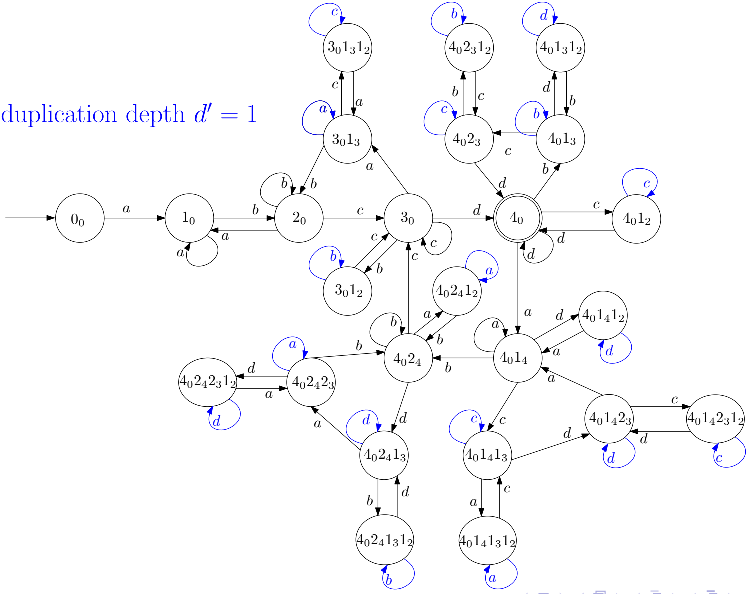
$\delta(q, y(q)[|y(q)|-d'+1]]) = q1_{d'}$

$\delta(q(j-1)_{d'}, y(q)[|y(q)|-d'+j]]) = qj_{d'}$,
where $2 \leq j \leq d'-1$

$\delta(q(d'-1)_{d'}, y(q)[|y(q)|]]) = q$

NFA Construction for $L(S)$

duplication depth $d' = 1$



NFA Construction for $L(S)$

Given a set $\mathcal{L}$ of possible duplication lengths,

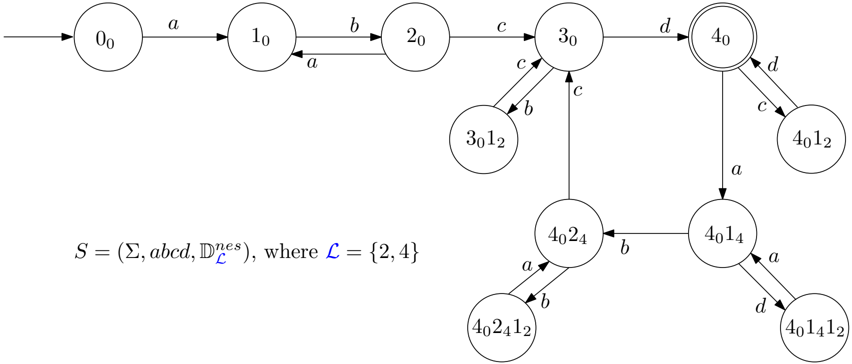


Figure: An example of NFA recognizing $L(S)$, where $S = (\Sigma, abcd, \mathbb{D}_{\mathcal{L}}^{nes})$.

NFA Construction for $L(S)$

Theorem

The NFA $M_S = (Q, \Sigma, \delta, 0_0, \{n_0\})$ recognizes the language generated by the nested duplication system $S = (\Sigma, s, \mathbb{D}^{nes}_{\leq k})$, $L(M_S) = L(S)$.

- **If $x \in L(S)$, then $x \in L(M_S)$.**
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If $x \in L(M_S)$, then $x \in L(S)$.

- For a string $x \in L(M_S)$, let p be the path that yields x.
- We recursively generate a series of paths p_i and strings x_i:
  1. p_1: generated by removing all self loops in p.
  2. ...
  3. p_i: generated by removing all cycles of size i in p_{i-1}.
- Then, $x_n = s$.

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Deduplication on finite automata!

Deduplication on Finite Automata

For a string $w' = xyyz$, where $|y| \leq k$, deduplication of w' transforms yy into y,

$$xyyz \rightarrow xyz.$$

$\mathbb{D}$-cycle deduplication

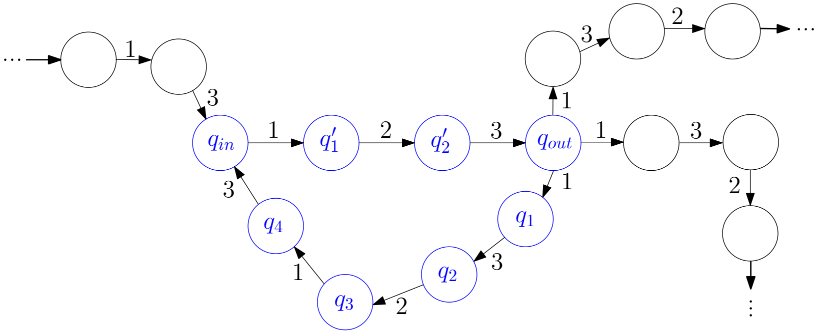
$\mathbb{D}$*-cycle deduplication* transforms a given NFA M to a smaller NFA M' while generating the same language in the duplication system by removing cycles in the NFA that satisfies special conditions,

$$L(S) = L(S'),$$

where $S = (\Sigma, L(M), \mathbb{D}^{nes}_{\leq k})$ and $S' = (\Sigma, L(M'), \mathbb{D}^{nes}_{\leq k})$.

$\mathbb{D}$-cycle deduplication

For a cycle C in an NFA, we call the cycle $\mathbb{D}$-*cycle* if C satisfies special conditions:



The cycle $C = (q_{in}, q'_1, q'_2, q_{out}, q_1, q_2, q_3, q_4, q_{in})$

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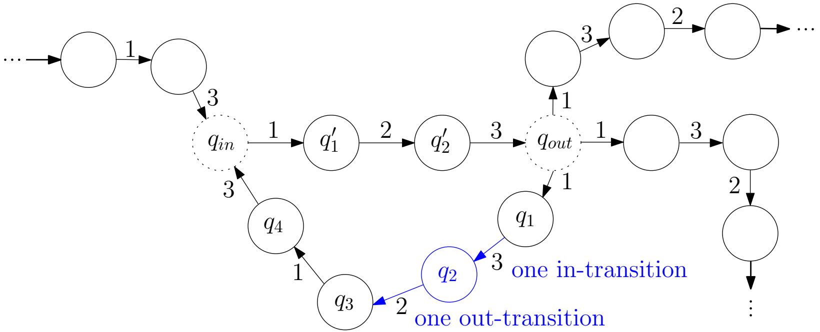

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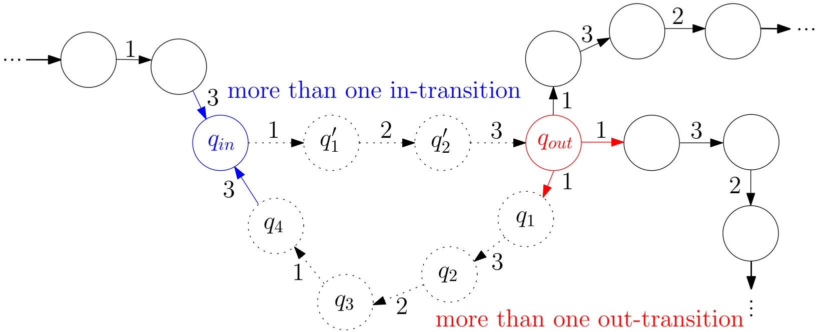

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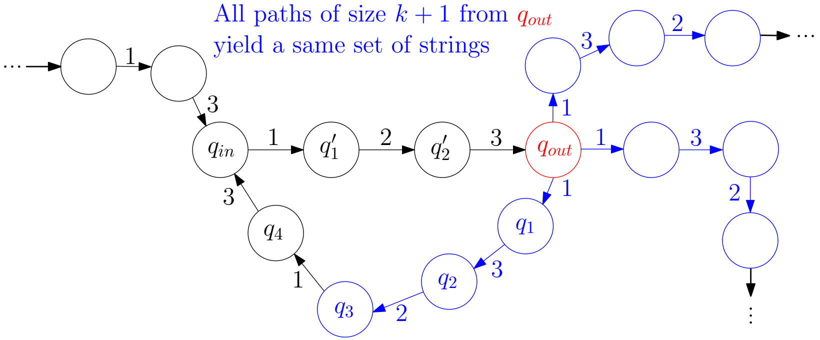

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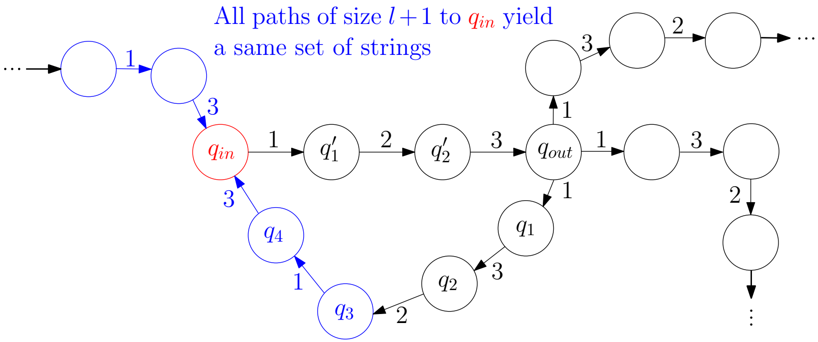

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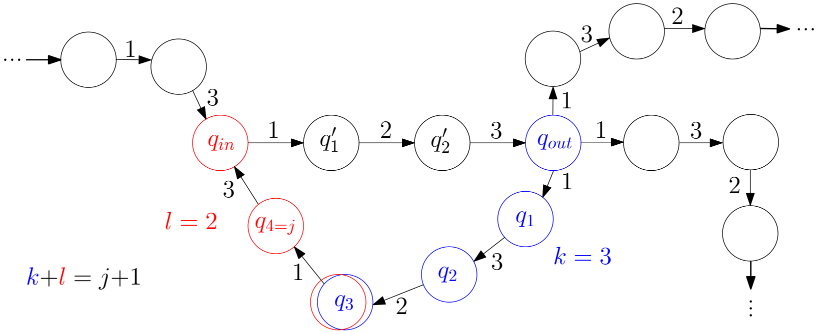

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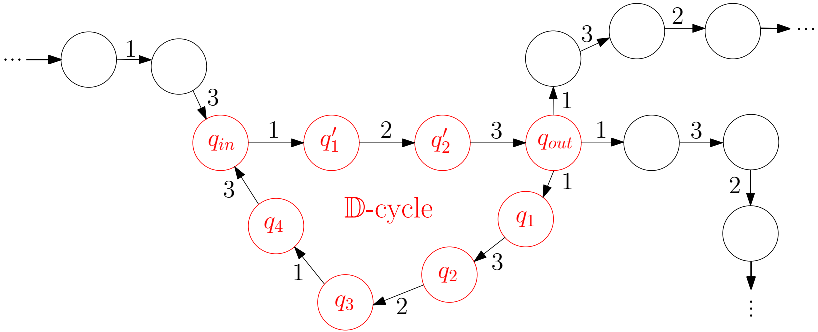


The $\mathbb{D}$-cycle $C = (q_{in}, q'_1, q'_2, q_{out}, q_1, q_2, q_3, q_4, q_{in})$

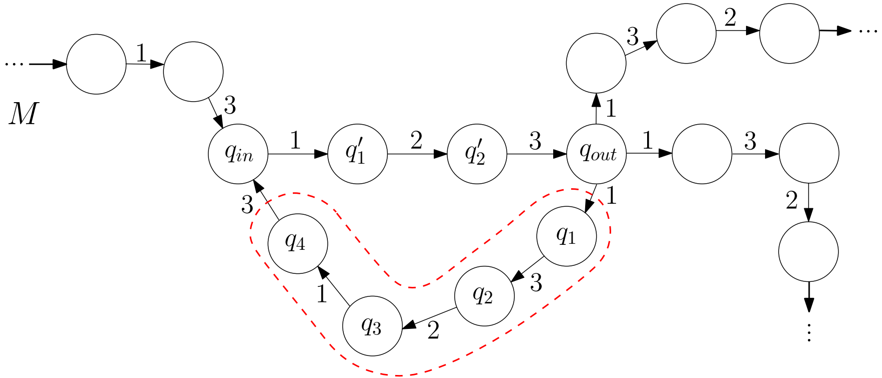
$\mathbb{D}$-cycle deduplication

Definition

Given an NFA $M = (Q, \Sigma, \delta, s, F)$ with a $\mathbb{D}$-cycle $(q_{in}, q'_1, q'_2, \ldots, q'_i, q_{out}, q_1, q_2, \ldots, q_j, q_{in})$, we define a $\mathbb{D}$-cycle deduplication by $M \xrightarrow{\mathbb{D}^{-1}_{\leq h}} M'$, where $i+j = h$, to be

$$M' = (Q \backslash \{q_1, q_2, \ldots, q_j\}, \Sigma, \{\delta(p, \alpha) = q \mid p, q \notin \{q_1, q_2, \ldots, q_j\}\}, s, F).$$

$\mathbb{D}$-cycle deduplication



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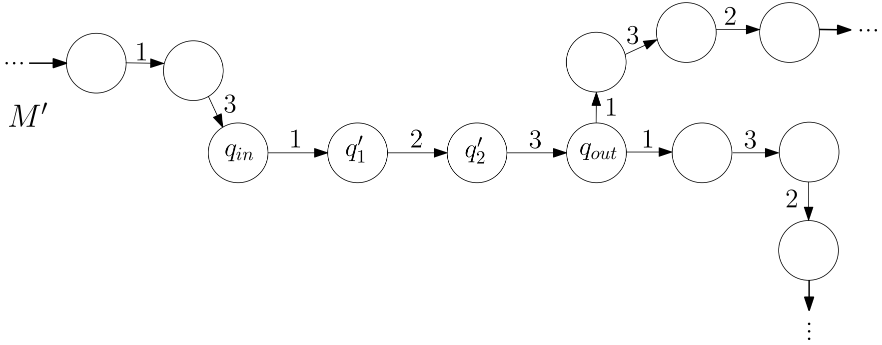


Lemma

Given an NFA M and its deduplication M′ such that $M \xrightarrow{\mathbb{D}^{-1}_{\leq h}} M'$*,*
let $S = (\Sigma, L(M), \mathbb{D}^{nes}_{\leq k})$ *and* $S' = (\Sigma, L(M'), \mathbb{D}^{nes}_{\leq k})$*. Then,*

$$L(S) = L(S').$$

NFA Construction for $L(S)$

Theorem

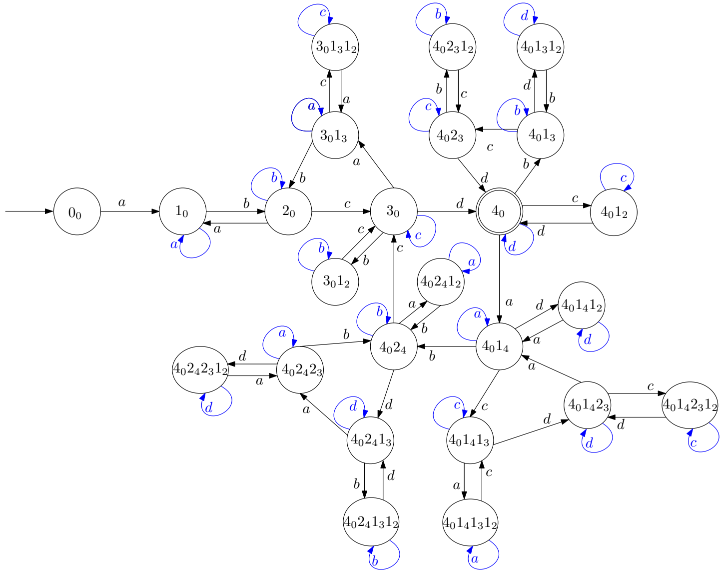
The NFA $M_S = (Q, \Sigma, \delta, 0_0, \{n_0\})$ recognizes the language generated by the nested duplication system $S = (\Sigma, s, \mathbb{D}^{nes}_{\leq k})$, $L(M_S) = L(S)$.

If $x \in L(M_S)$, then $x \in L(S)$.

- For a string $x \in L(M_S)$, let p be the path that yields x.
- We recursively generate a series of paths p_i and strings x_i:
  1. p_1: generated by removing all self loops in p.
  2. ...
  3. p_i: generated by removing all cycles of size i in p_{i-1}.
- Then, $x_n = s$.

Deduplication on finite automata!

NFA Construction for $L(S)$



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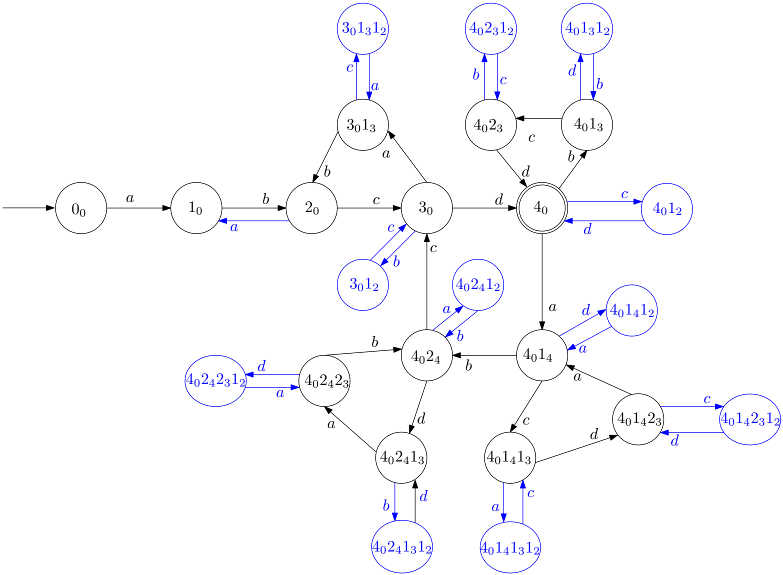

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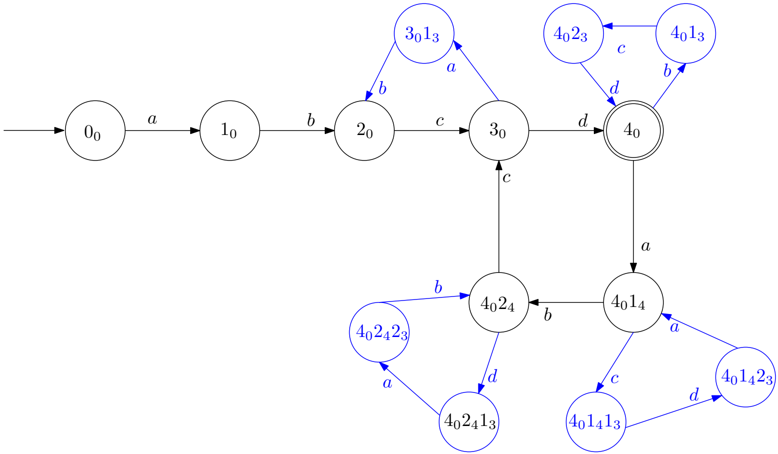

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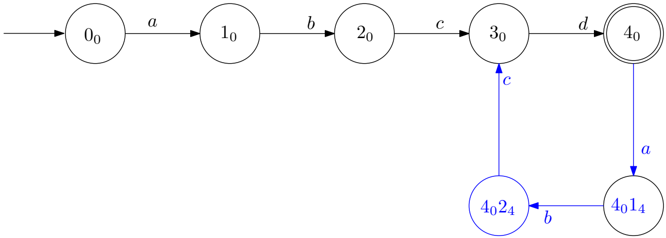

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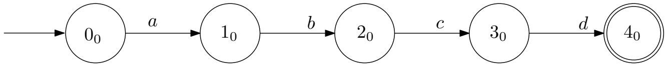

Computing the Capacity of S

Definition

The *capacity* of a duplication system S represents how many strings the system produces compared to Σ^n, where n goes to infinity,

$$cap(S) = \lim_{n\to\infty} \sup \frac{\log_{|\Sigma|} |S \cap \Sigma^n|}{n}.$$

From Jain et al. (2015), it is known that we can compute the capacity of S represented by DFA using Perron-Frobenius Theory.

Computing the Capacity of S

1. Construct an NFA M_S for $S = (\Sigma, s, \mathbb{D}^{nes}_{\leq k})$.
2. Convert M_S to a DFA M'.
3. Find the maximal connected component in M' and compute its adjacency matrix $\mathbb{M}$.
4. Return the maximum eigenvalue of $\mathbb{M}$ using Perron-Frobenius Theory.

Summary

- Defined
  - the nested duplication operation $\mathbb{D}^{nes}_{\leq k}(w)$,
  - the nested duplication system $S(\Sigma, s, \mathbb{D}^{nes}_{\leq k})$.
- Presented an NFA construction for L of $S(\Sigma, s, \mathbb{D}^{nes}_{\leq k})$
- Introduced the $\mathbb{D}$-cycle deduplication on NFA

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Thank you!