COUNTING, GENERATING AND SAMPLING TREE ALIGNMENTS

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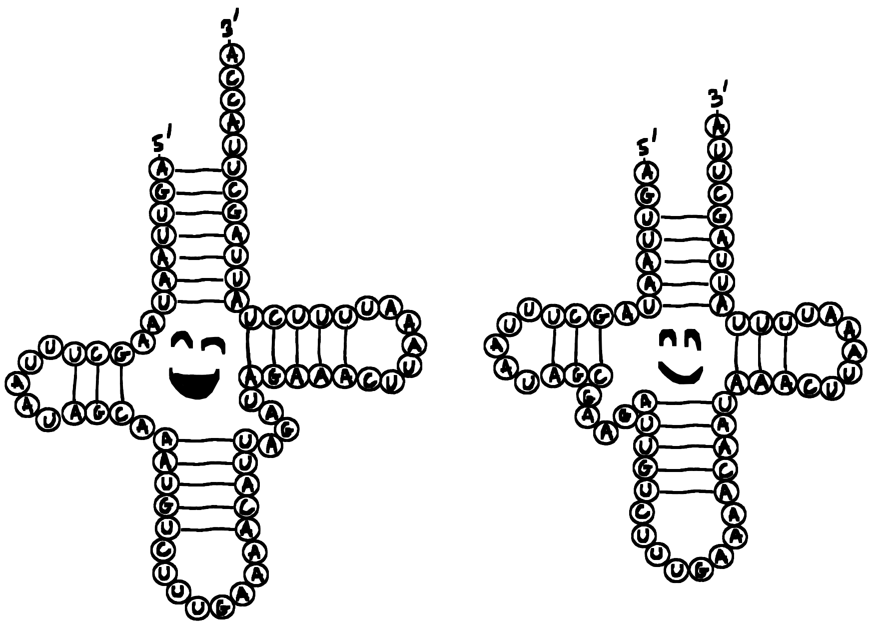
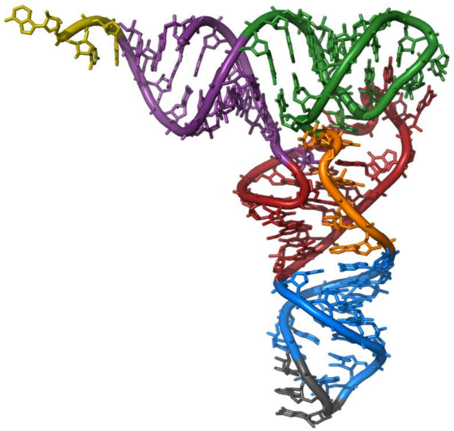
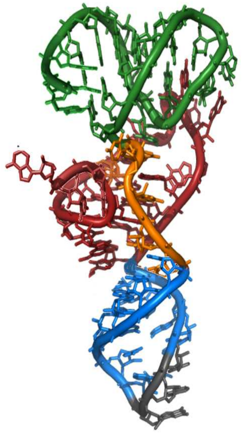


Lille, January 5th 2015

MOTIVATION: RNA COMPARISON

Question: how to measure similarity between two RNAs?





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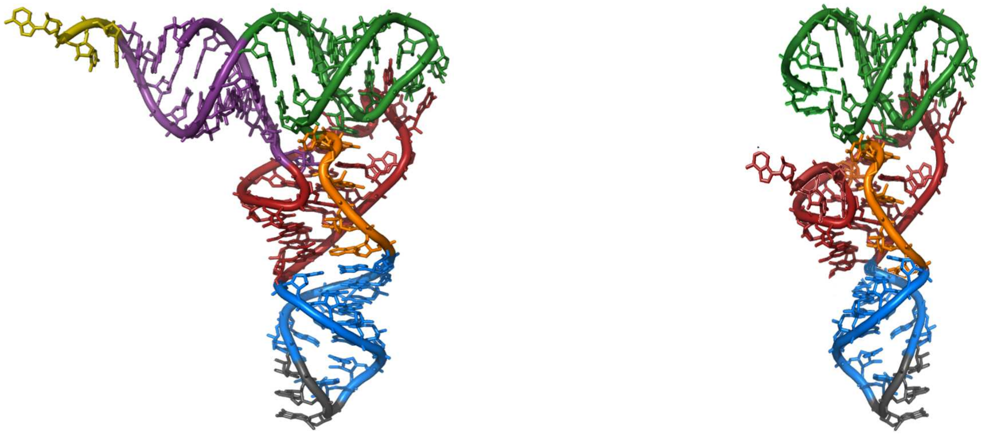

First idea: compare nucleic acid sequences.

RNA 1: A U U C G A U U A ...

RNA 2: A C C A U G A U U A ...

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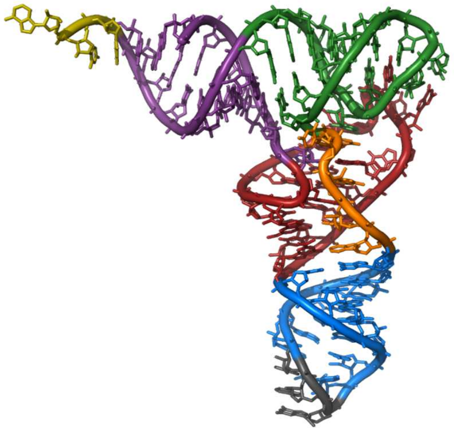

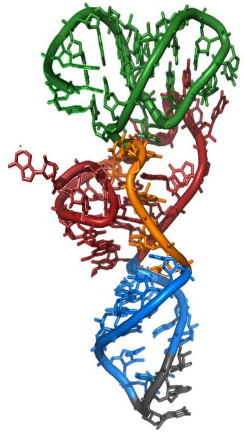

First idea: compare nucleic acid sequences.

→ sequence alignment

RNA 1: A U U C G A U U A ...

RNA 2: A C C A U G A U U A ...

alignment: $\begin{pmatrix}A\\A\end{pmatrix}\begin{pmatrix}U\\-\end{pmatrix}\begin{pmatrix}-\\C\end{pmatrix}\begin{pmatrix}U\\-\end{pmatrix}\begin{pmatrix}C\\C\end{pmatrix}\begin{pmatrix}-\\A\end{pmatrix}\begin{pmatrix}-\\U\end{pmatrix}\begin{pmatrix}G\\G\end{pmatrix}\begin{pmatrix}A\\A\end{pmatrix}\begin{pmatrix}U\\U\end{pmatrix}\begin{pmatrix}U\\U\end{pmatrix}\begin{pmatrix}A\\A\end{pmatrix}\ldots$

MOTIVATION: RNA COMPARISON

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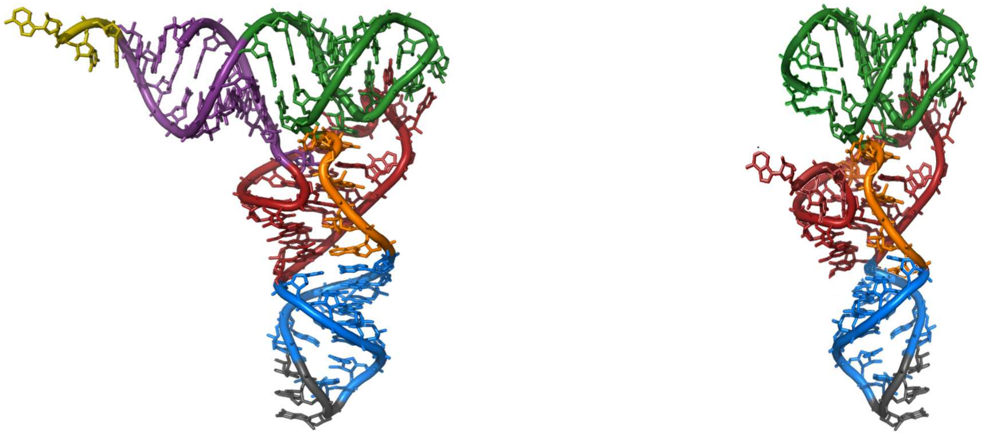
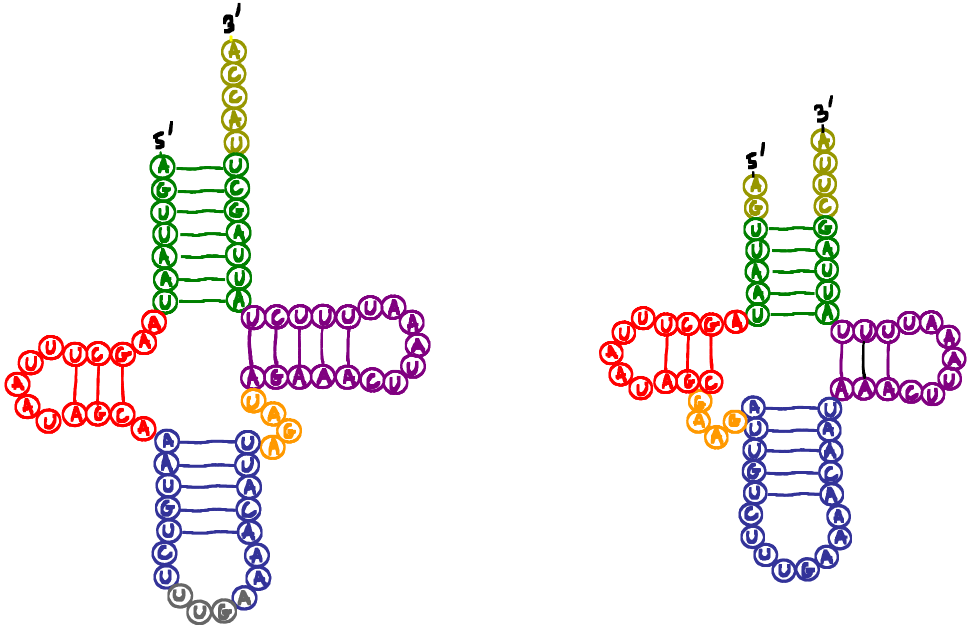
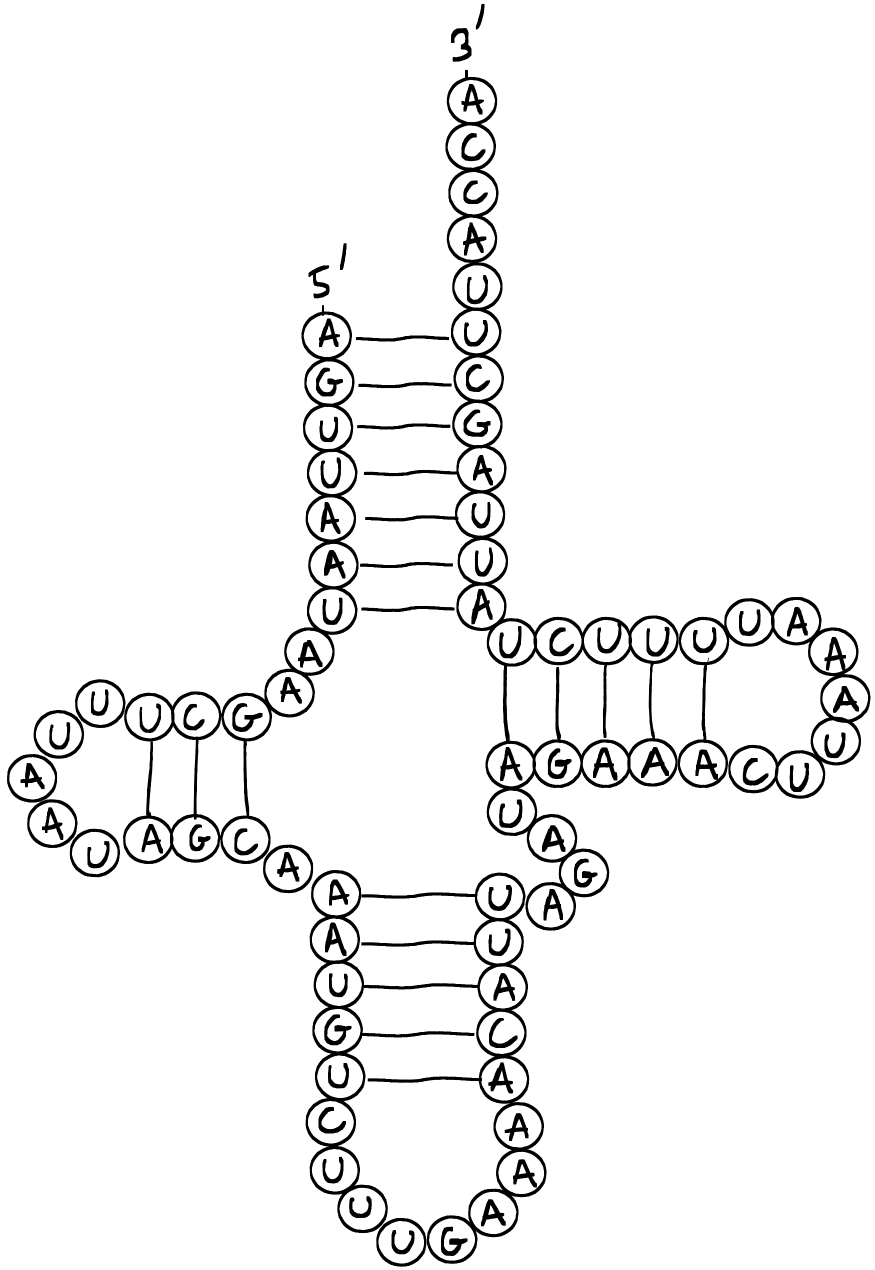


Second idea: compare secondary structures.



→ notion of tree alignment [Jiang, Wang, Zhang]

FROM SECONDARY STRUCTURES TO TREES



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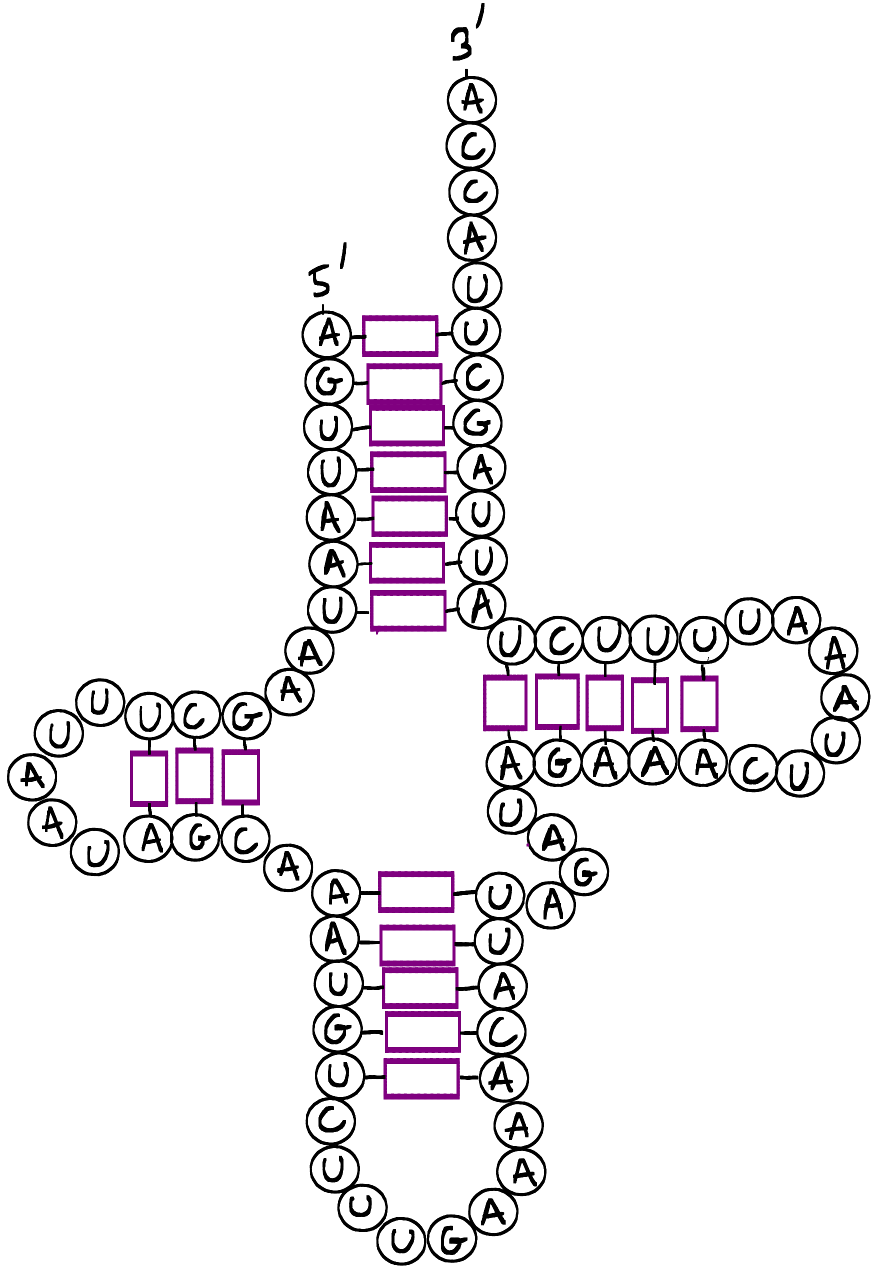

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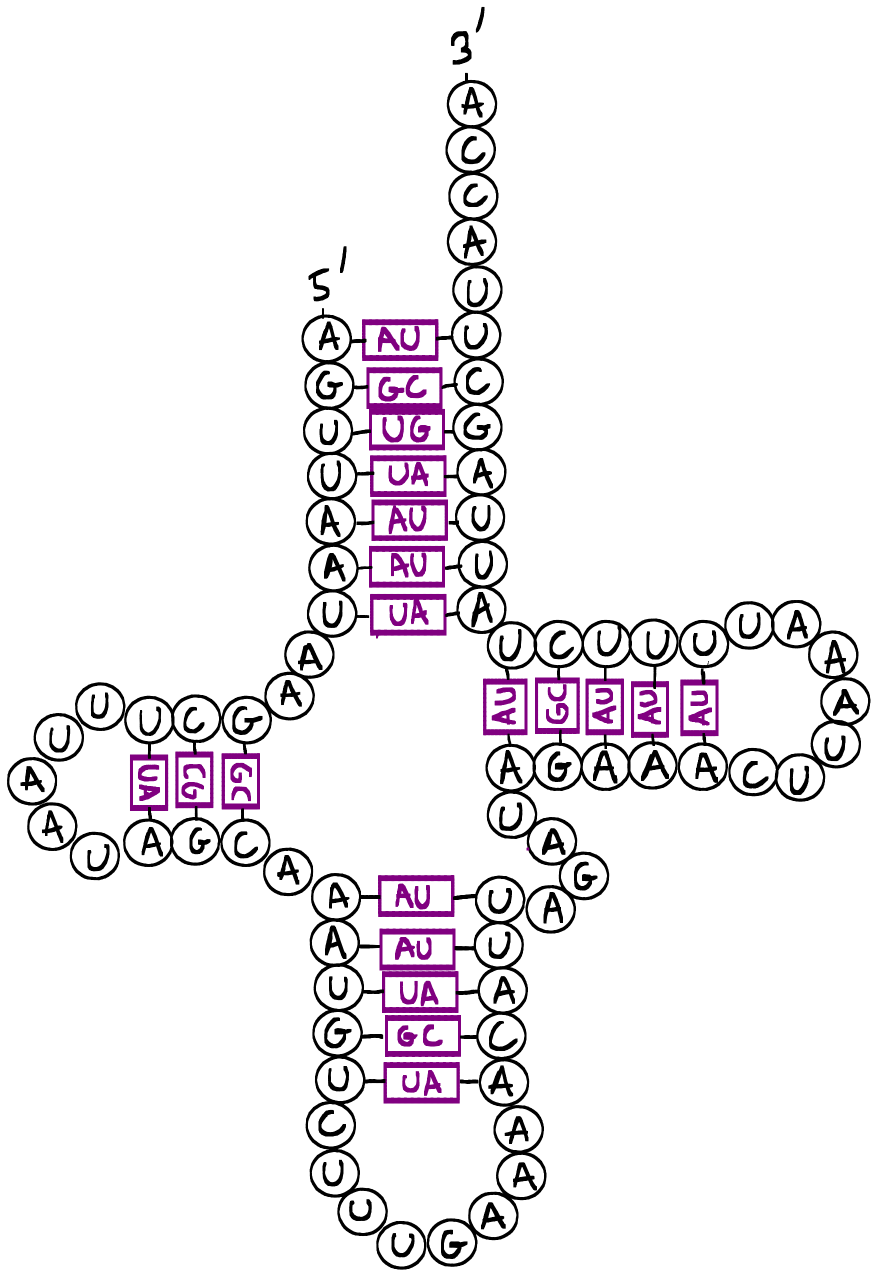

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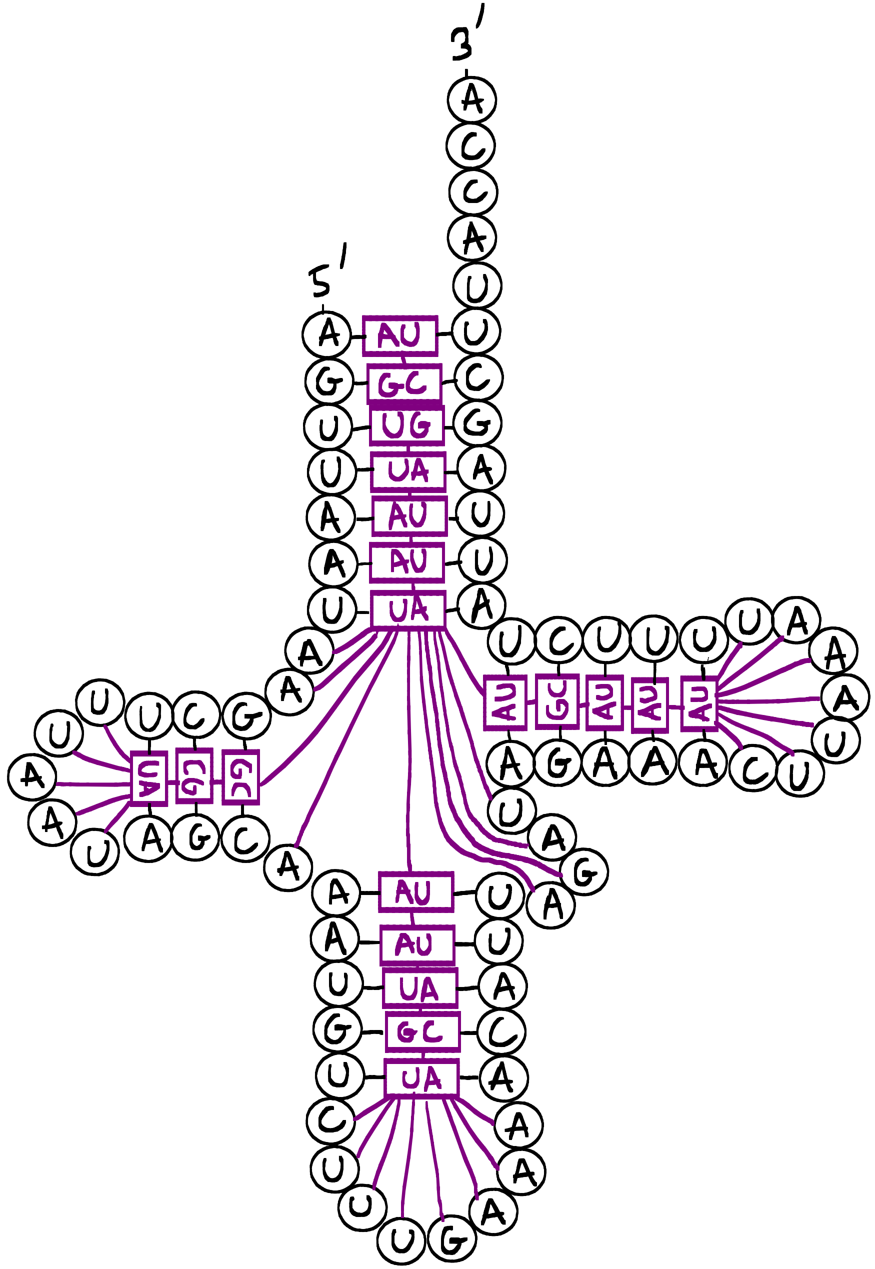

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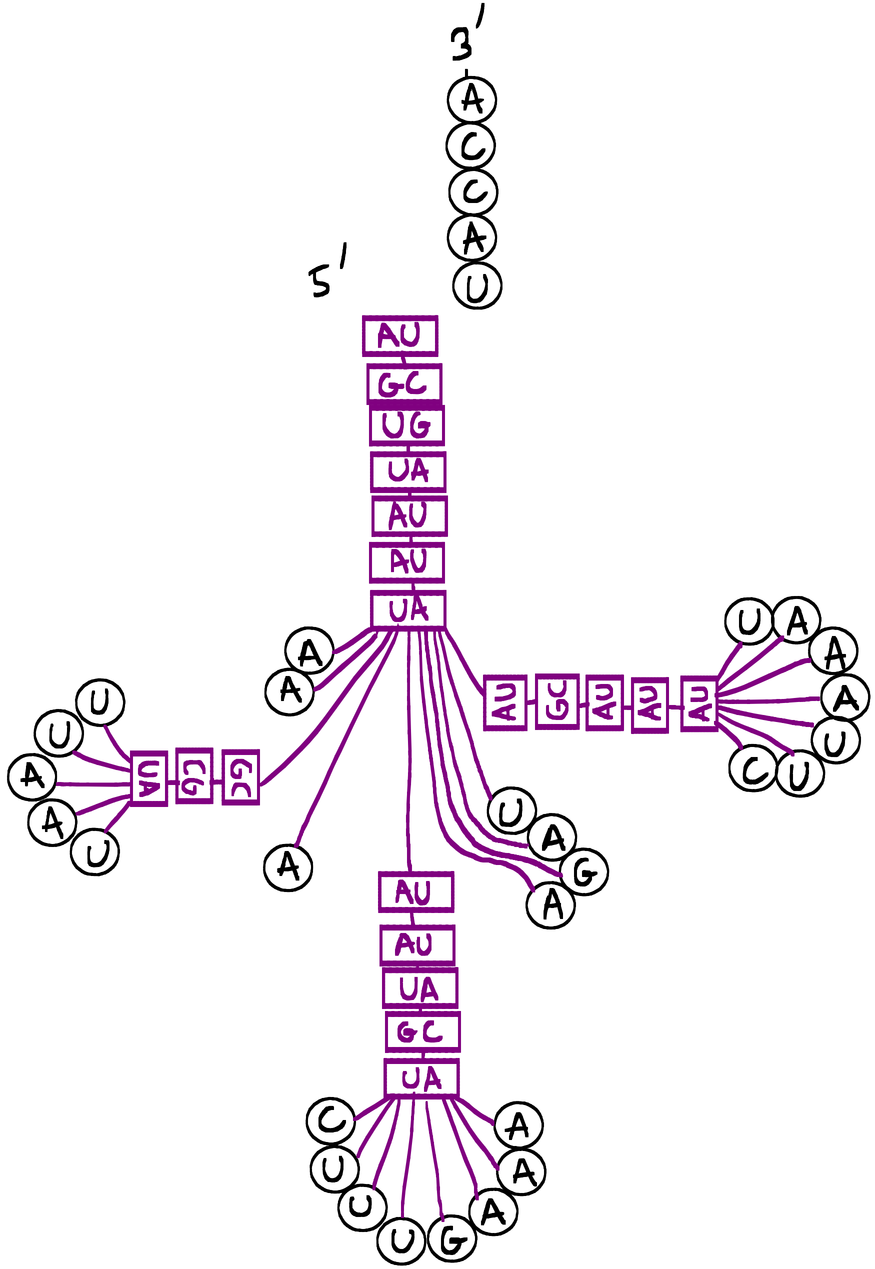

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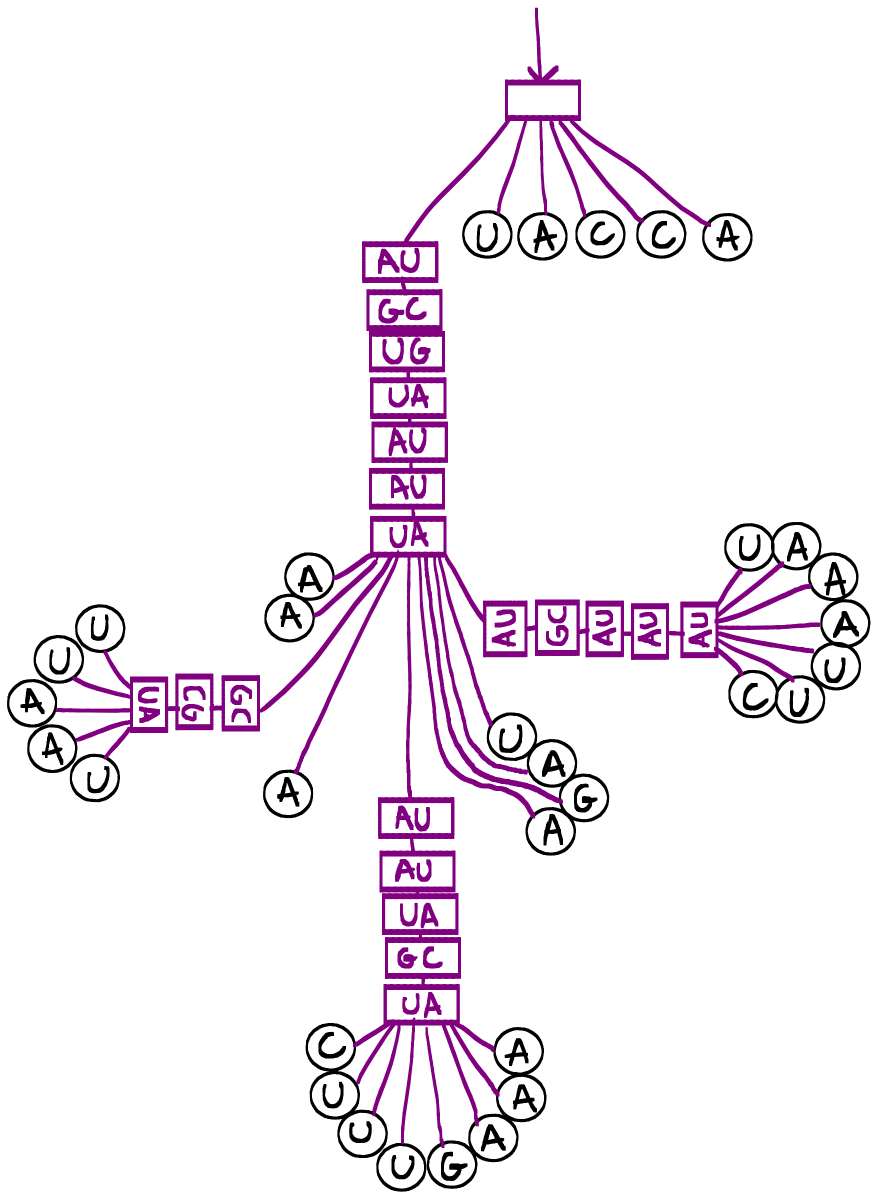
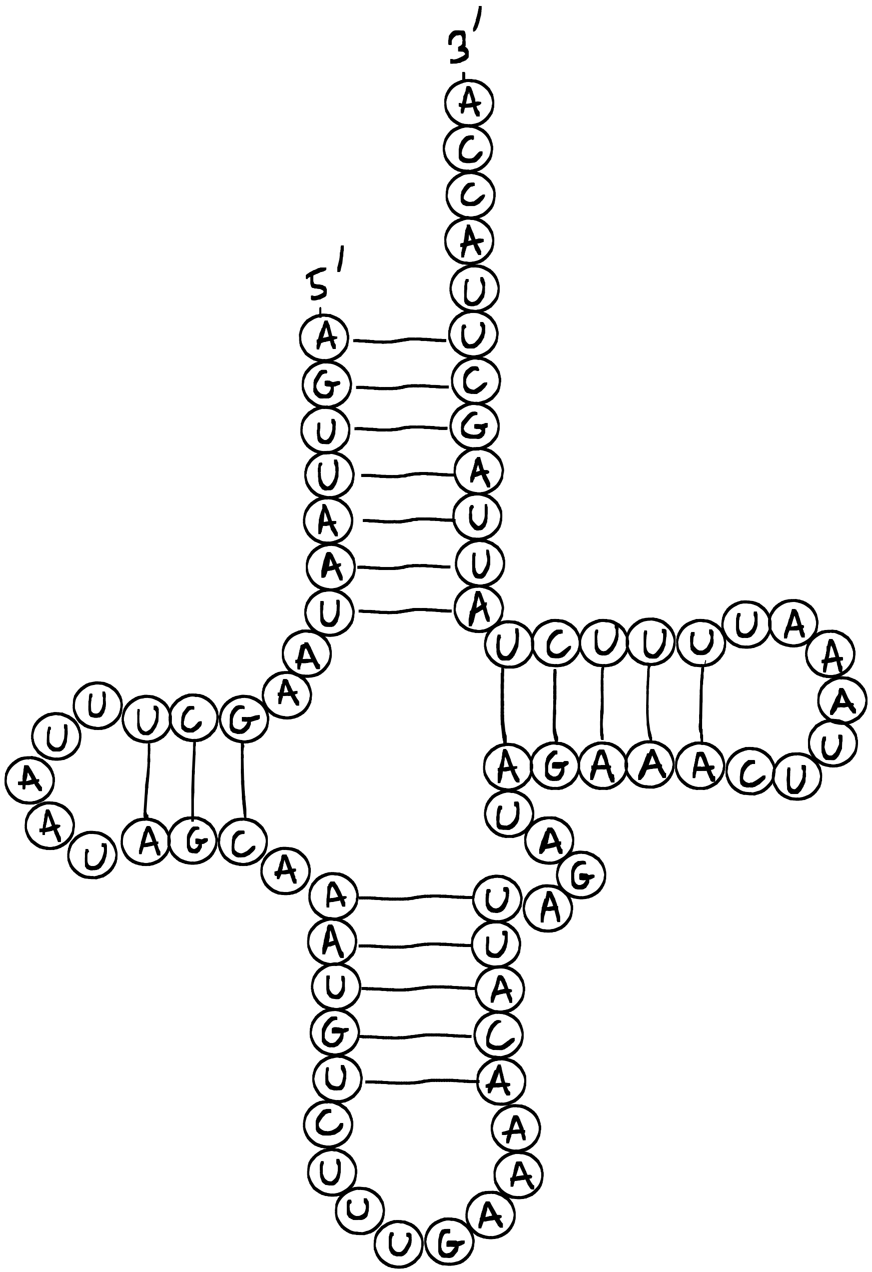
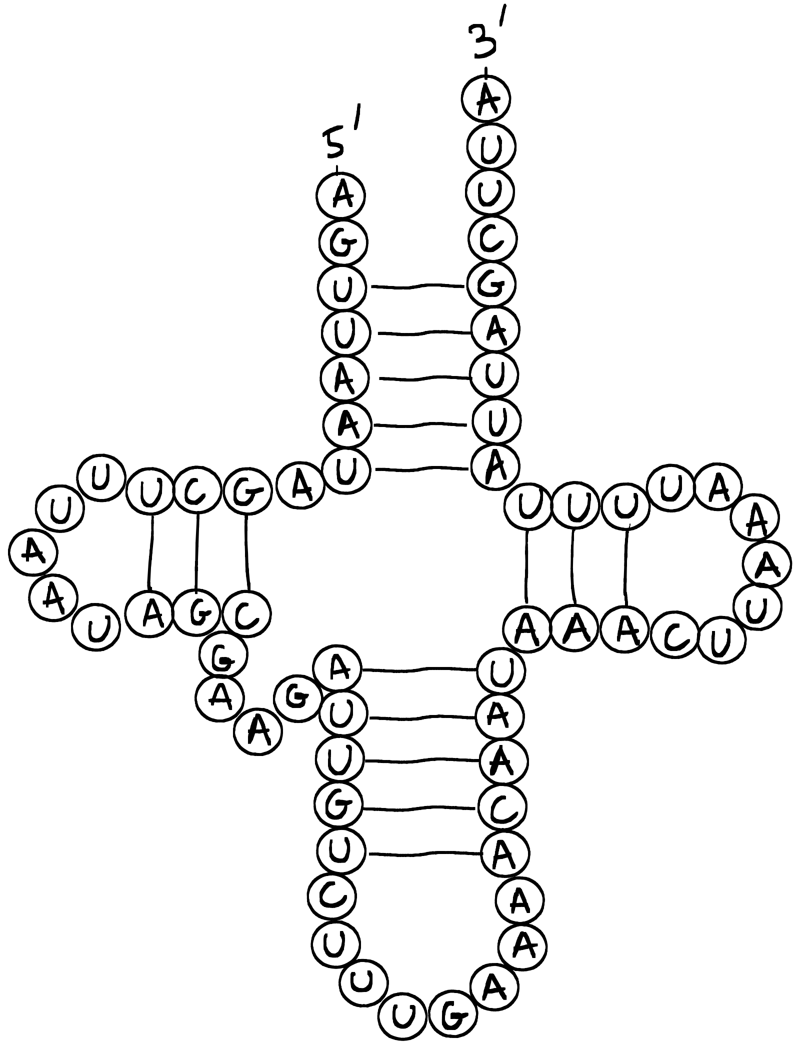


FROM SECONDARY STRUCTURES TO TREES

Objective: Align trees coming from RNA 2^{ary} structures





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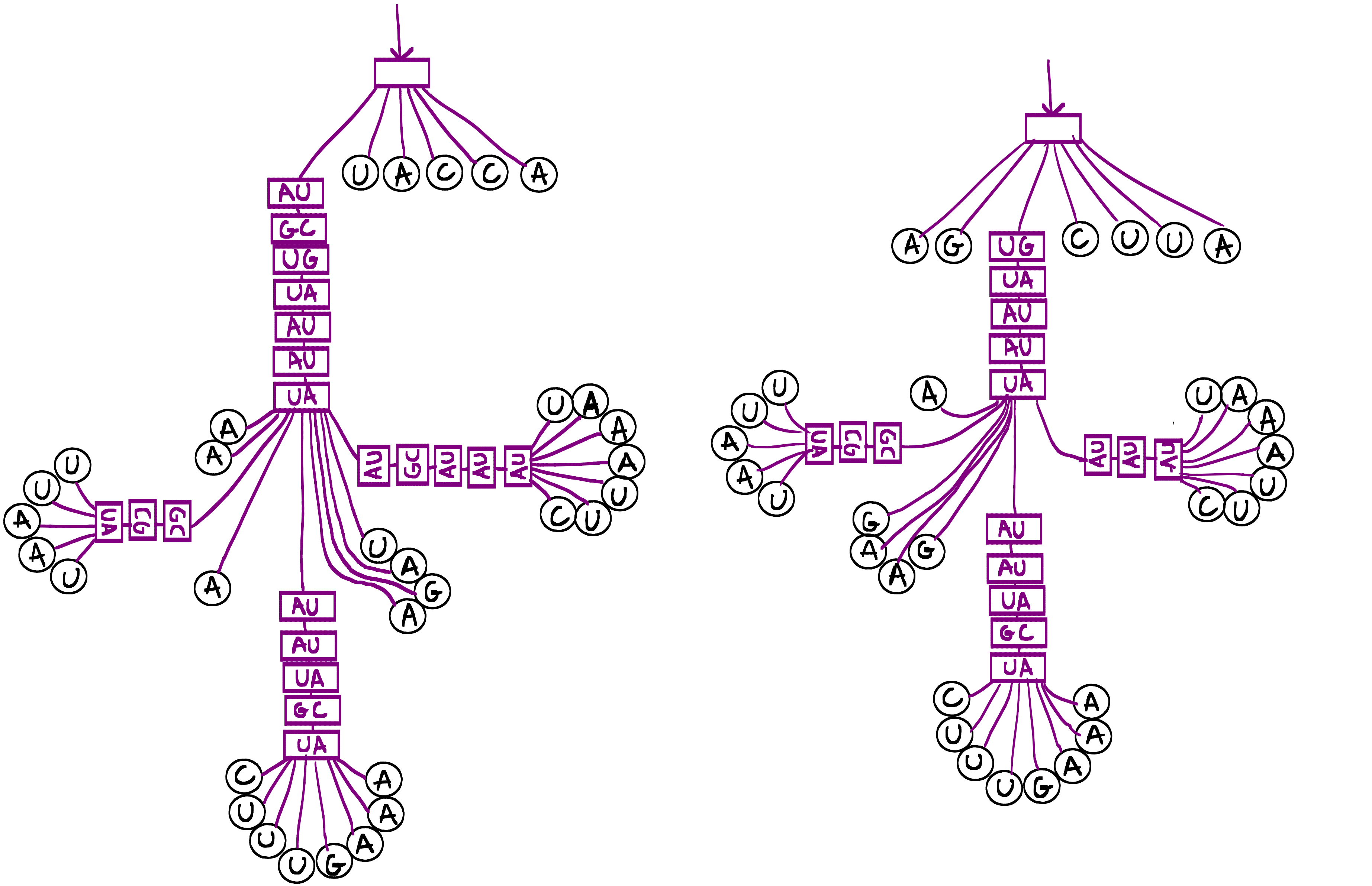
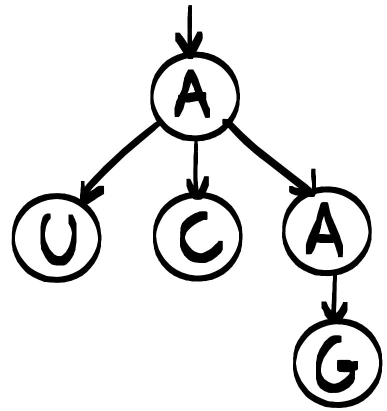


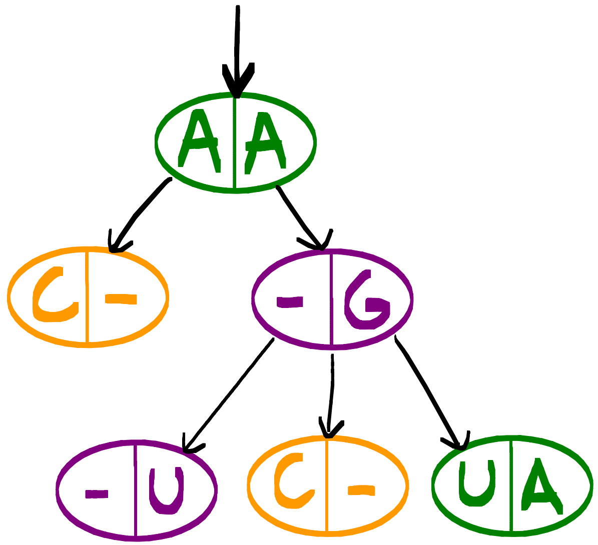
TREES AND SUPERTREES

Trees are plane, rooted,
and vertices are labeled
by an alphabet Σ.



Supertree = tree with
3 types of vertices:

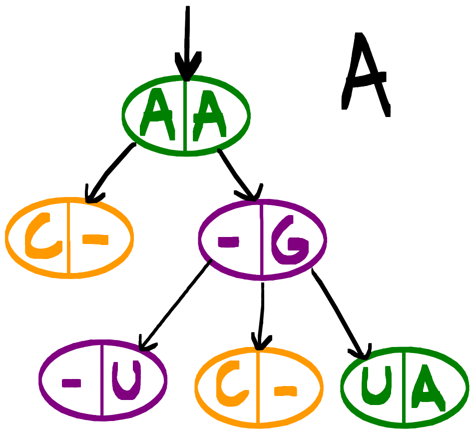
- X | Y (mis)match
- X | - insertion
- - | Y deletion



SUPERTREES INDUCE TREE ALIGNMENTS

Let A be a supertree,

$\pi_1(A)$ = tree
obtained by changing
X|Y → X
X|- → X
and removing -|Y.



$\pi_2(A)$ = tree
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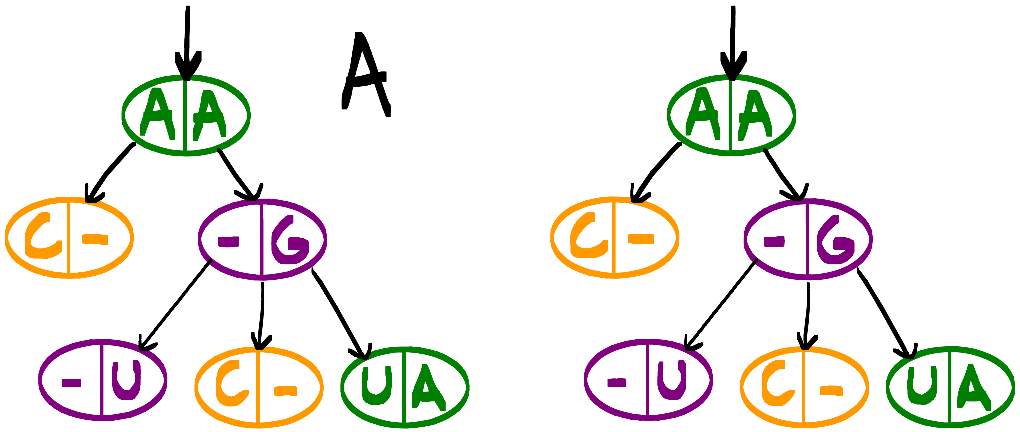

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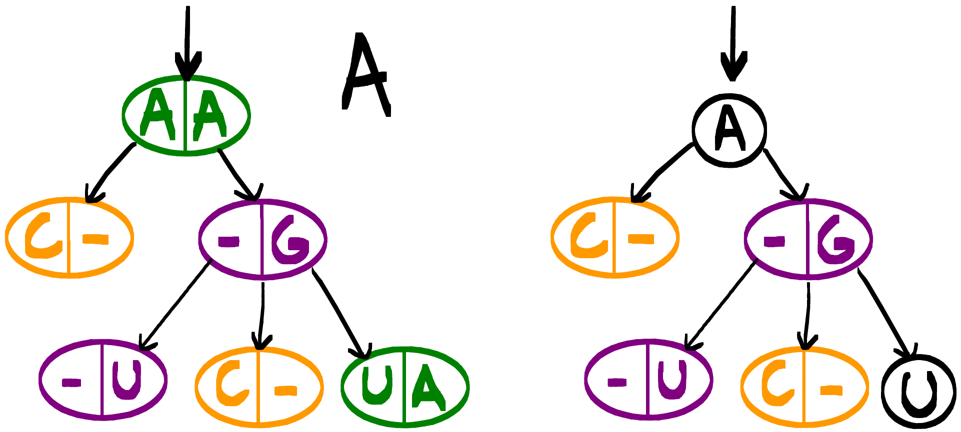

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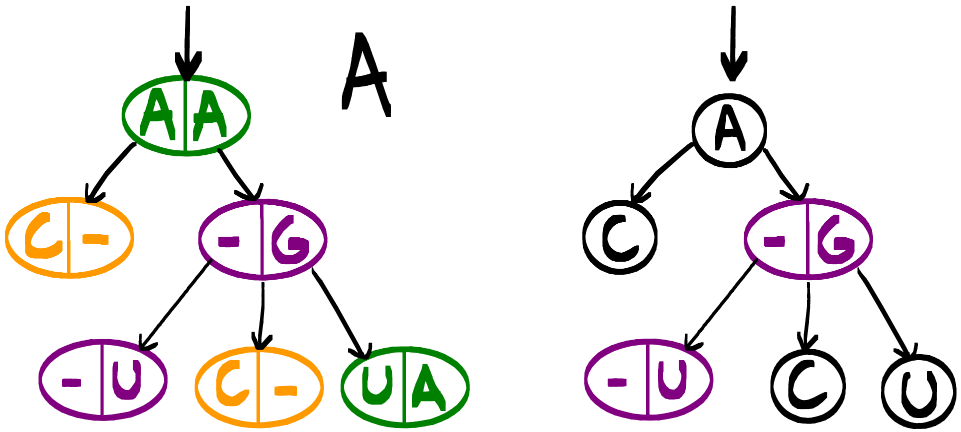

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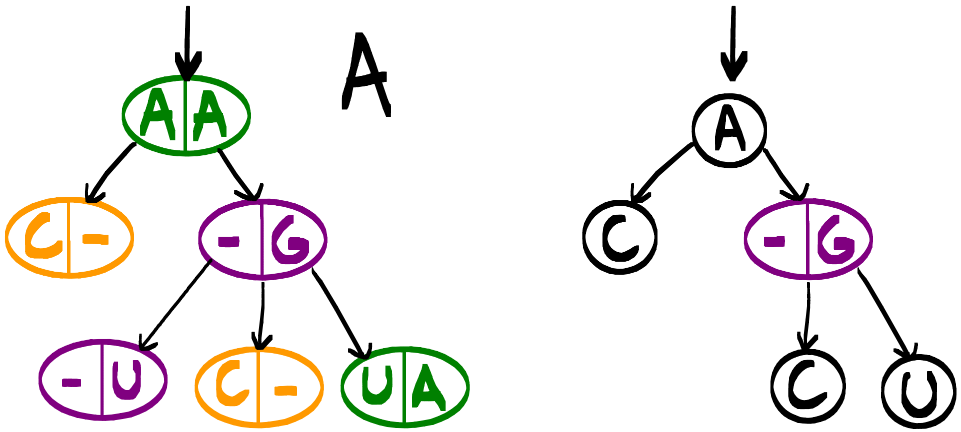

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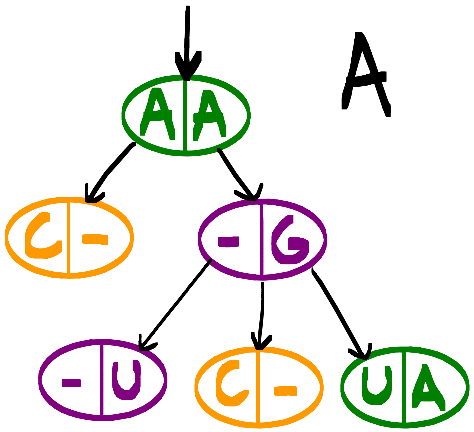

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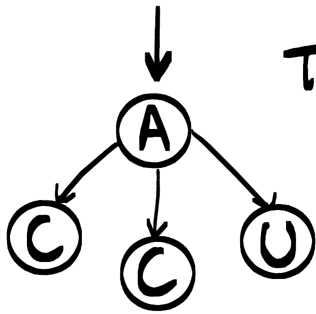

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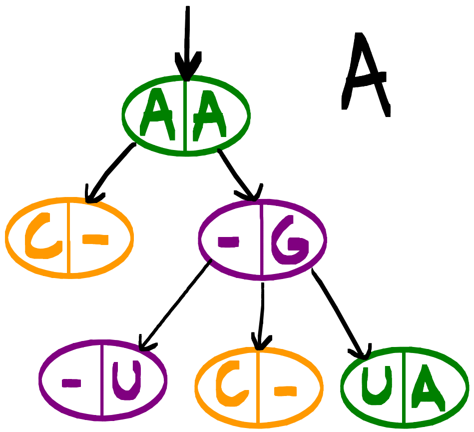

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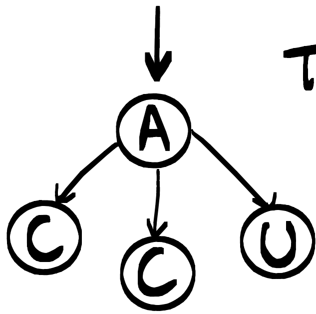

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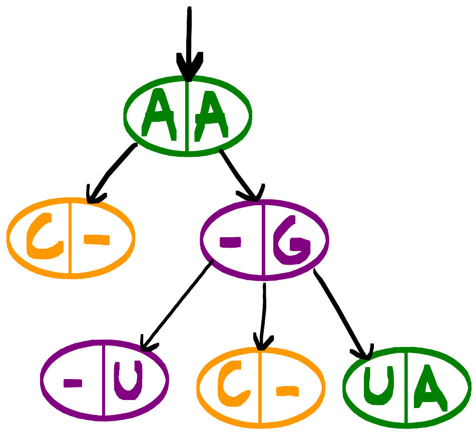

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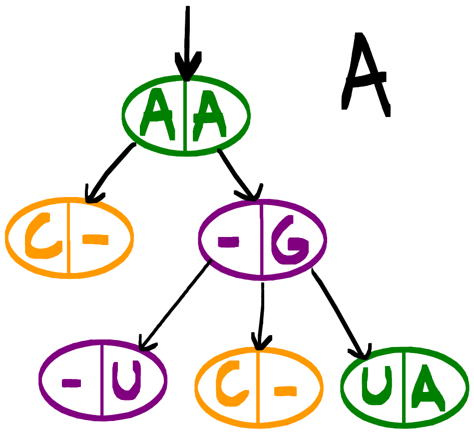

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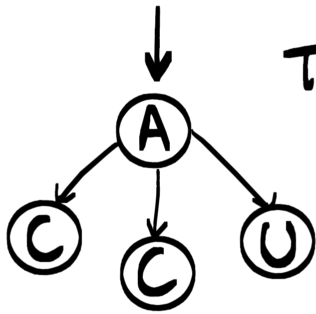

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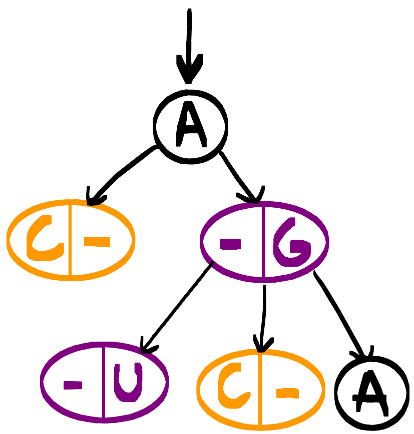

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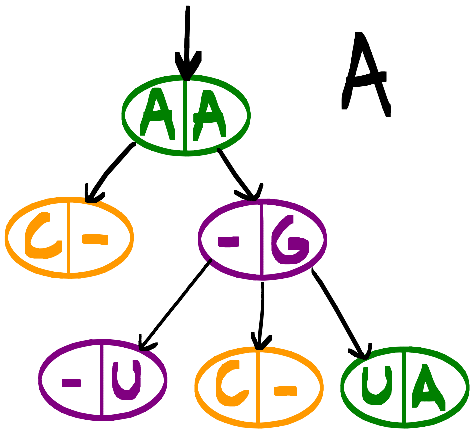

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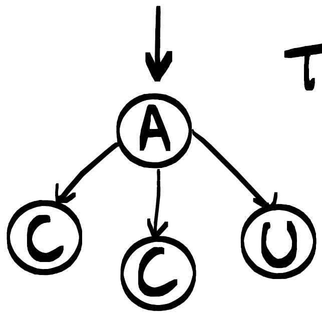

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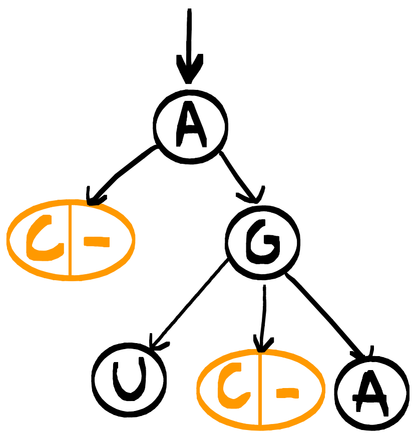

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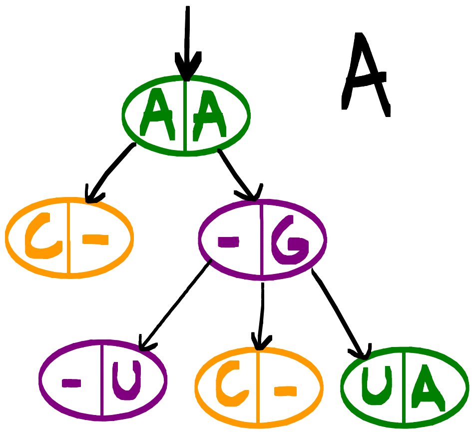

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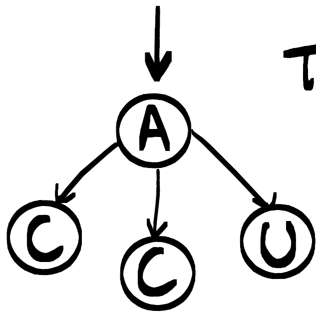

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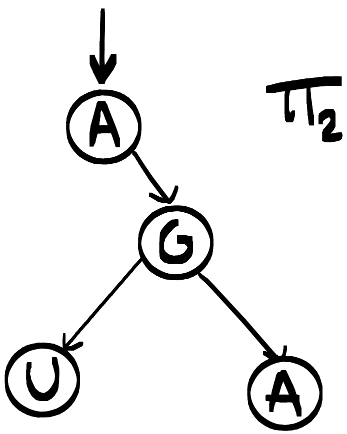
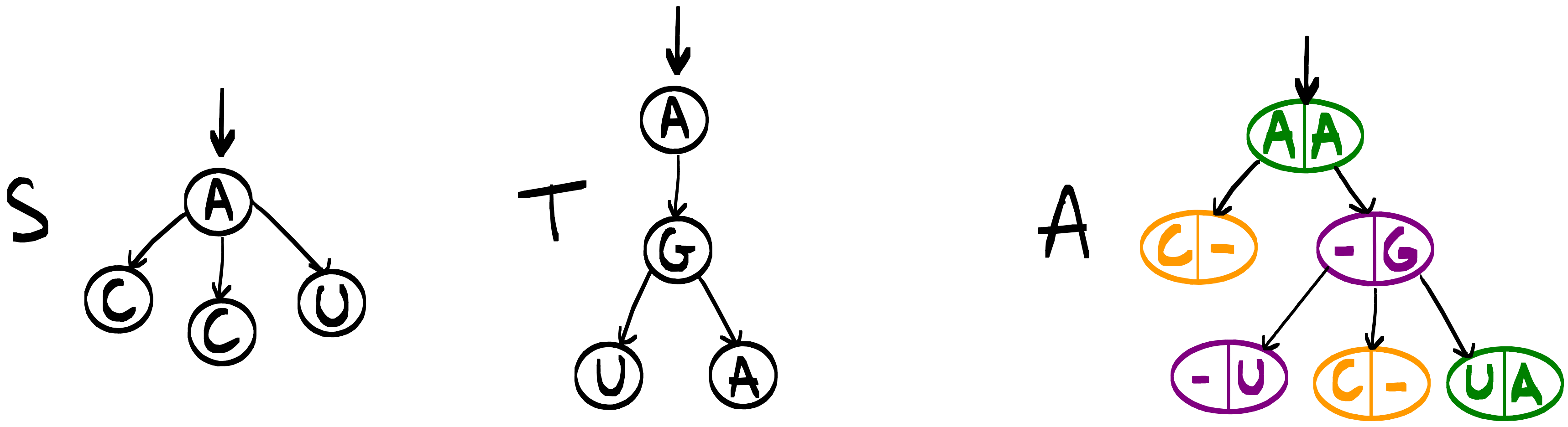


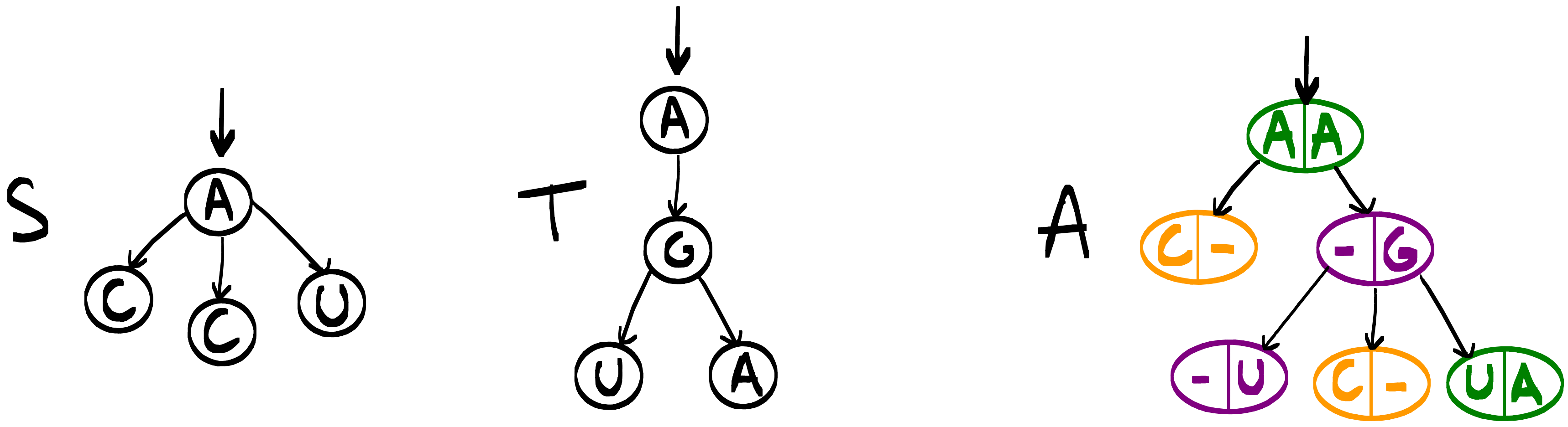
$\pi_2(A)$

SUPERTREES INDUCE TREE ALIGNMENTS



Given two trees S and T,
a supertree A defines an alignment between S and T
if $\pi_1(A) = S$ and $\pi_2(A) = T$.

SUPERTREES INDUCE TREE ALIGNMENTS



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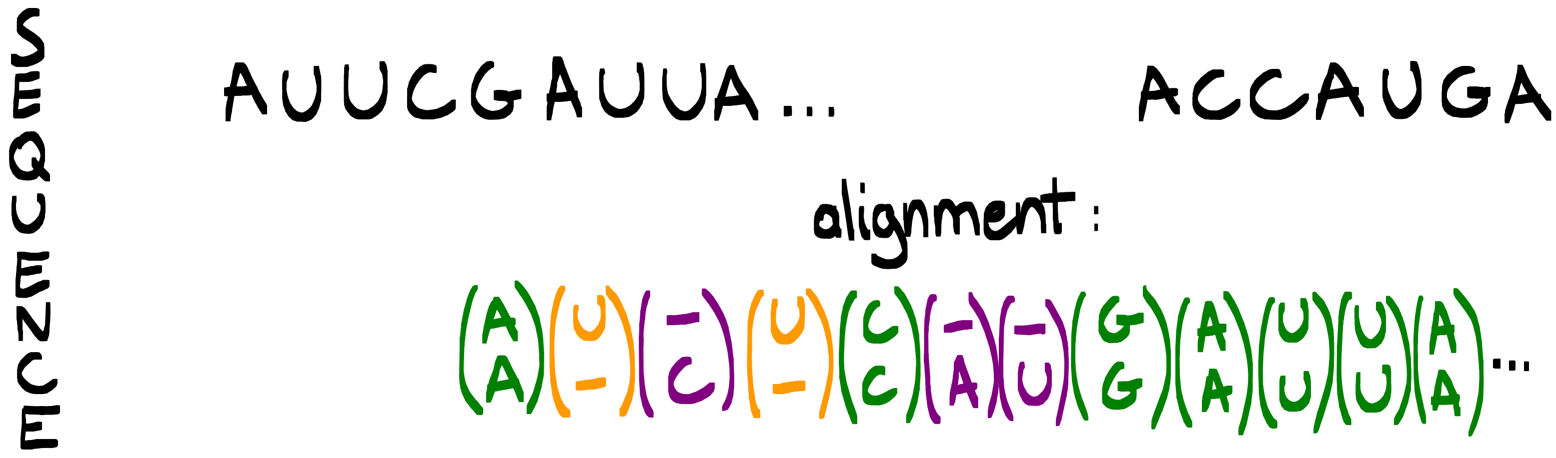
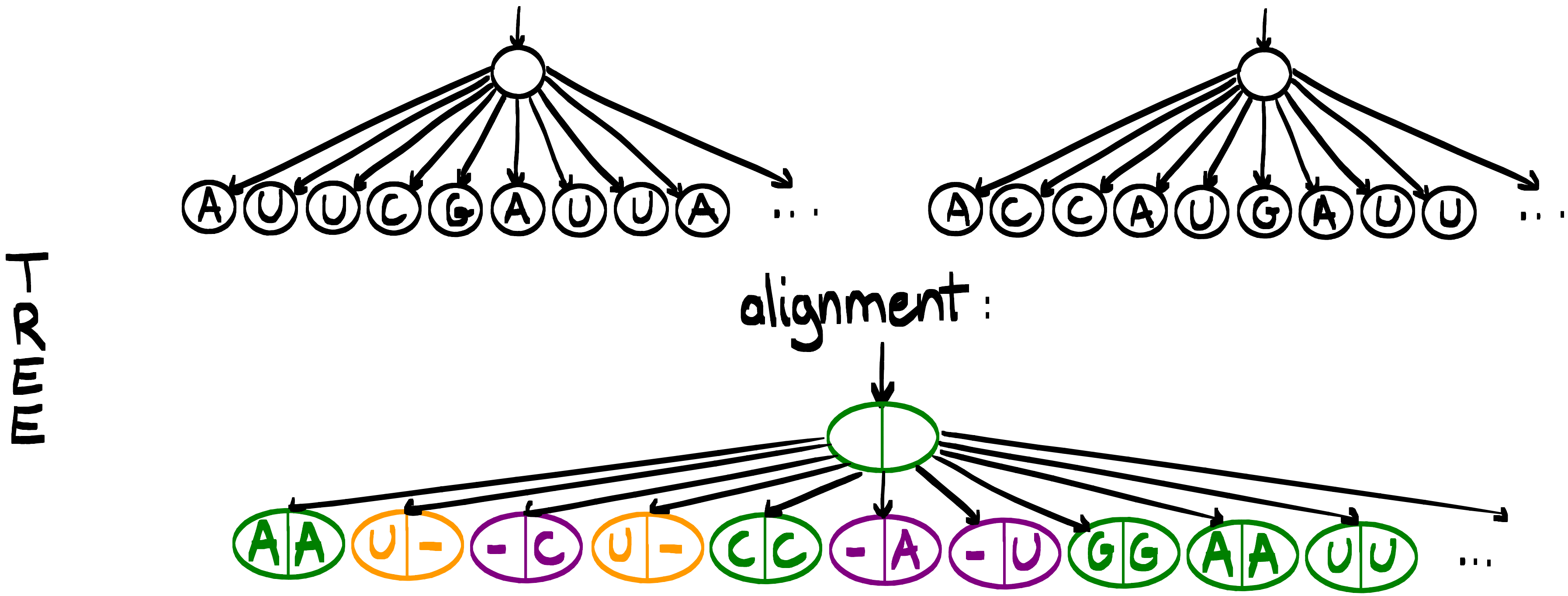
$\text{cost}(A)$ = nb of insertions + deletions + mismatches

(can be changed more complicated models)

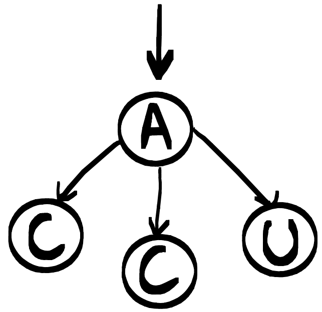
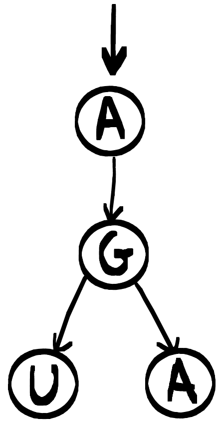
CONNECTION WITH SEQUENCE ALIGNMENTS

Tree alignments generalize sequence alignments.





SPACE OF ALIGNMENTS

Which alignment between  and 

is the most likely?

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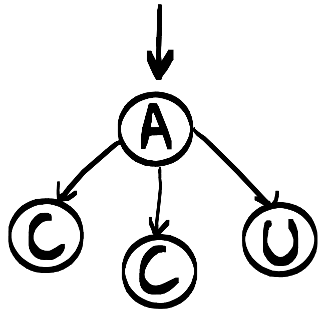

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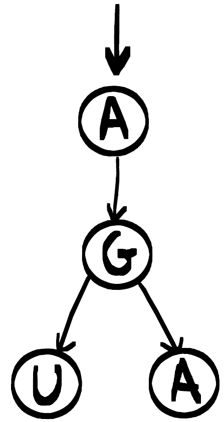

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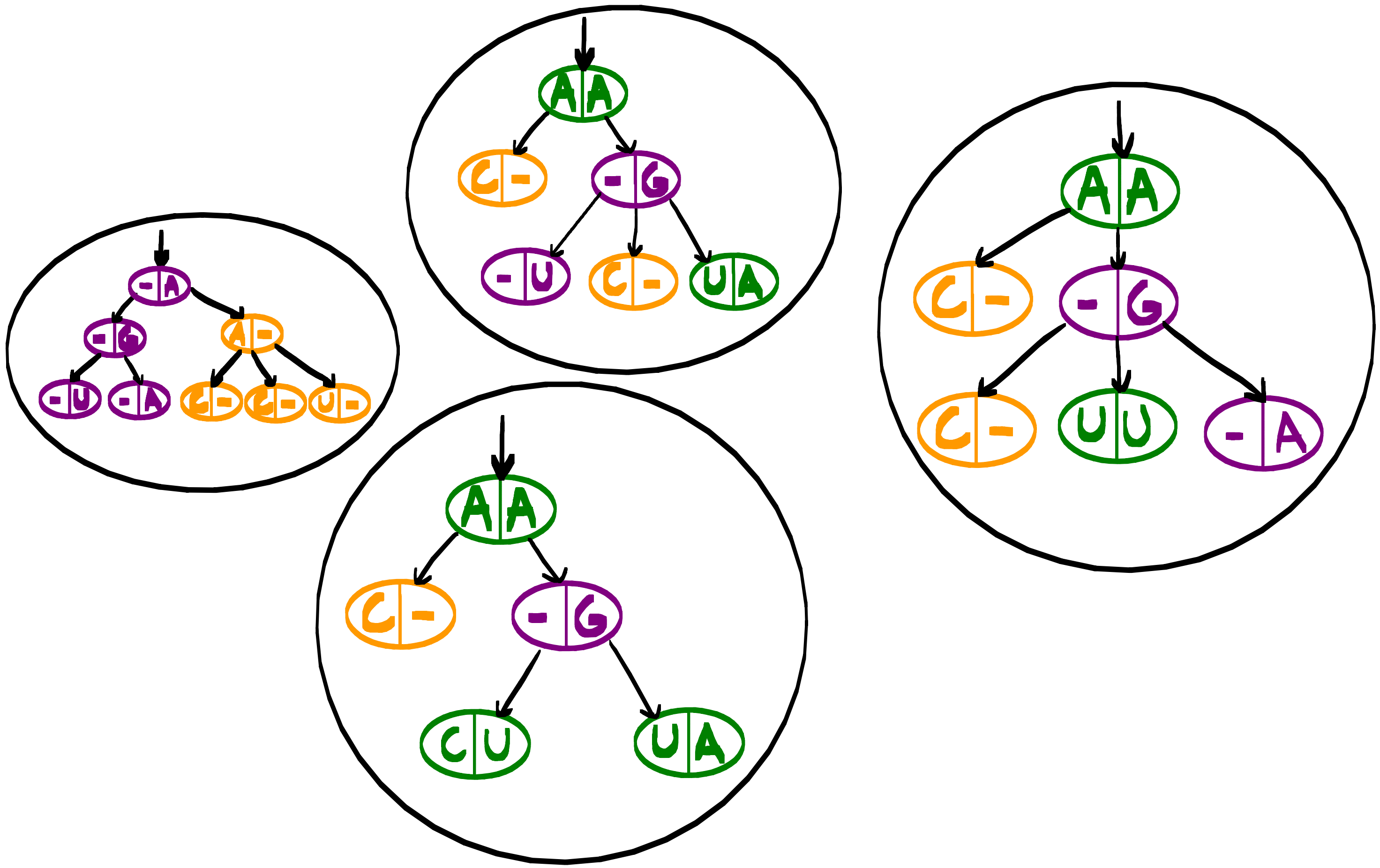

probability of an alignment A

$$\propto e^{-\frac{\mathrm{cost}(A)}{K}}$$

(Gibbs-Boltzmann distribution)

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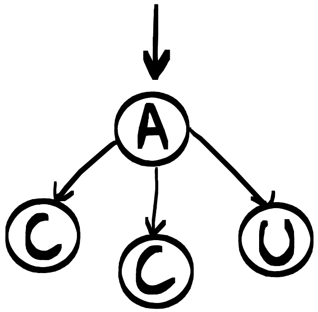
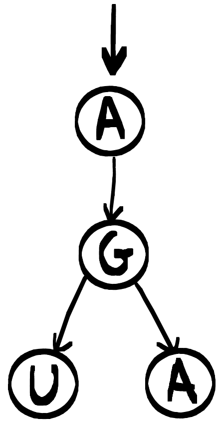
Which alignment between  and  is the most likely?

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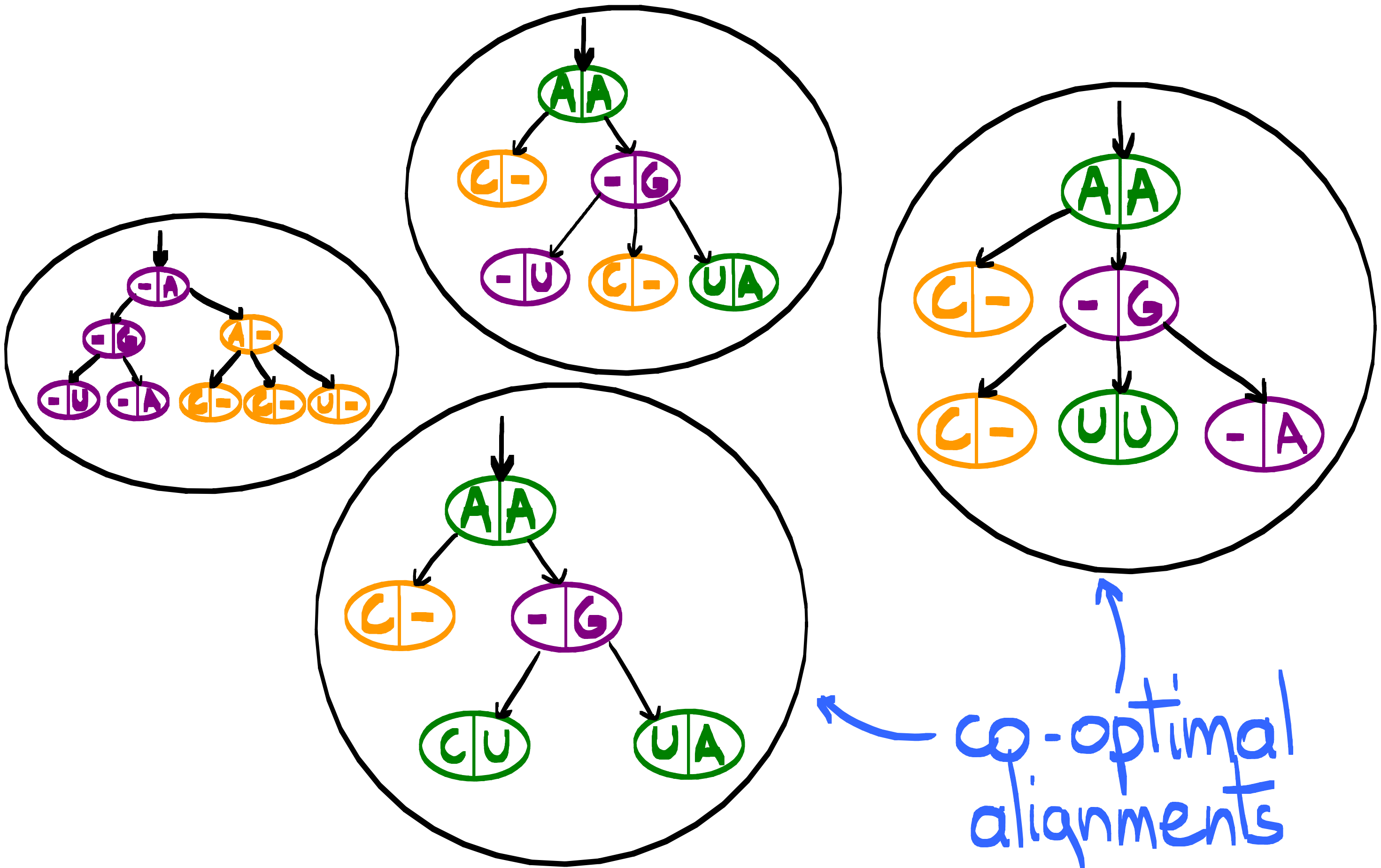

SPACE OF ALIGNMENTS

Why finding one optimal alignment may be inadequate:

- Co-optimal alignments can be very different.
  (see for instance [Vingron, Argos, 1990])

- Exploring the space of alignments enables the detection of high probability features.

SPACE OF ALIGNMENTS

Objective: Sampling alignments under the Gibbs-Boltzmann probability distribution.

probability of an alignment A

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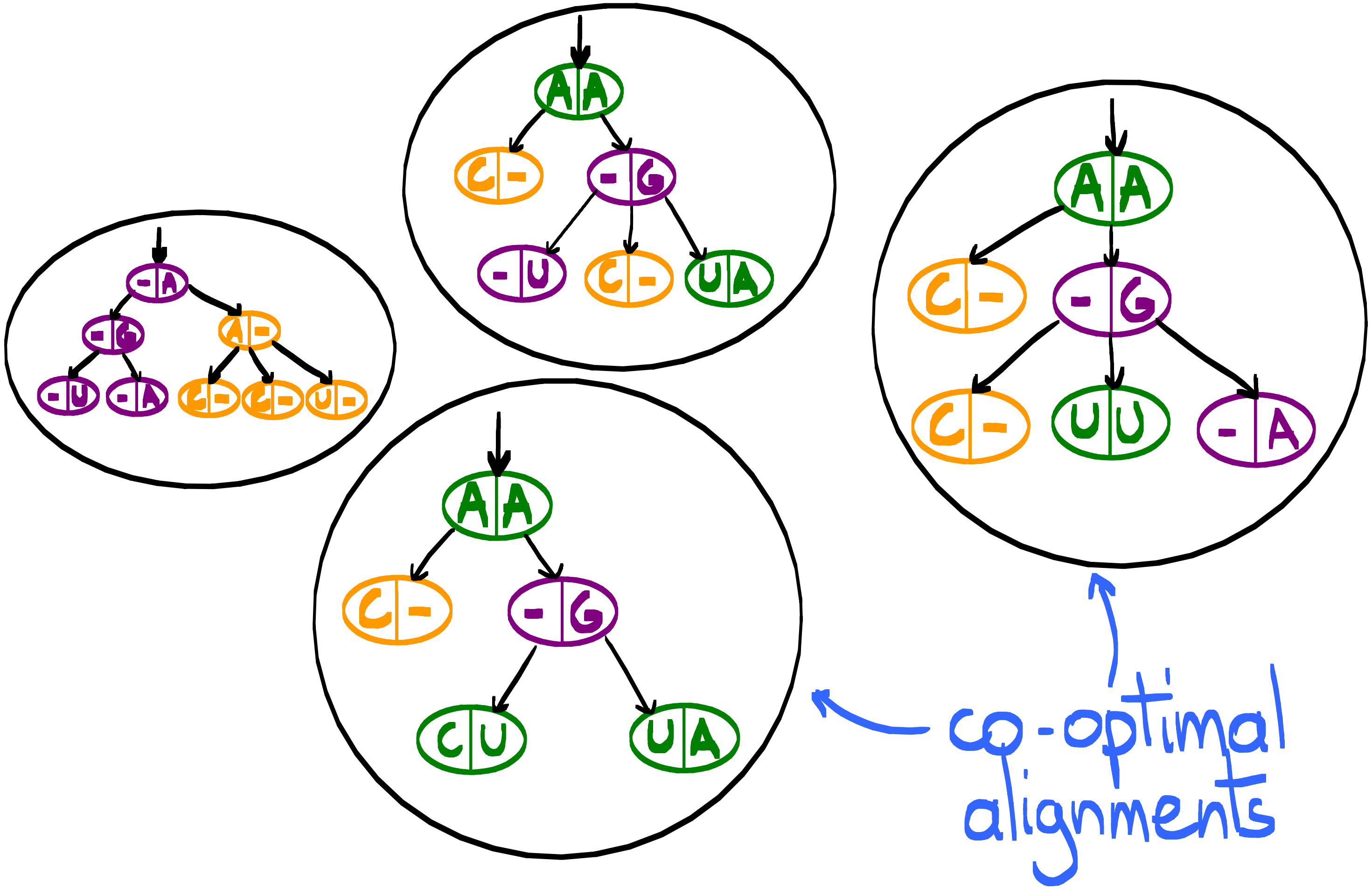

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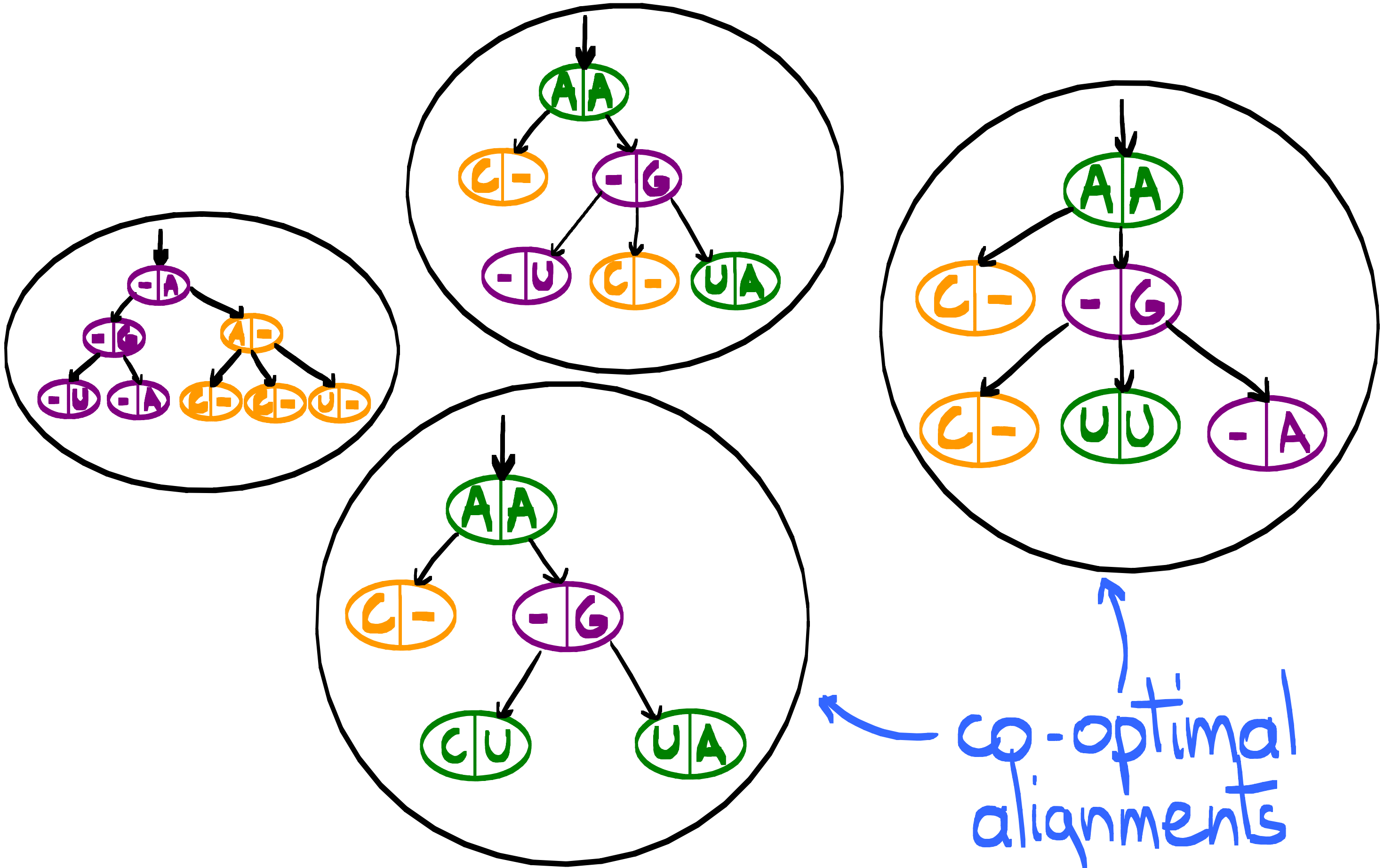
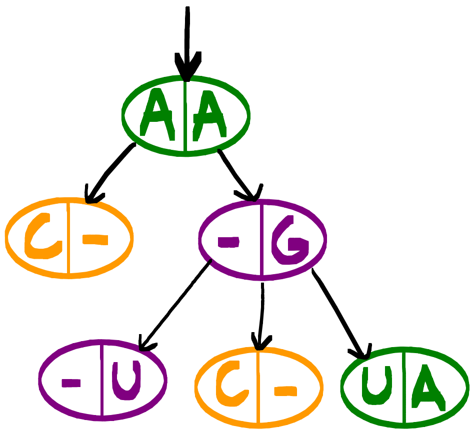
probability of an alignment A $\propto e^{-\frac{cost(A)}{K}}$ (Gibbs-Boltzmann distribution)

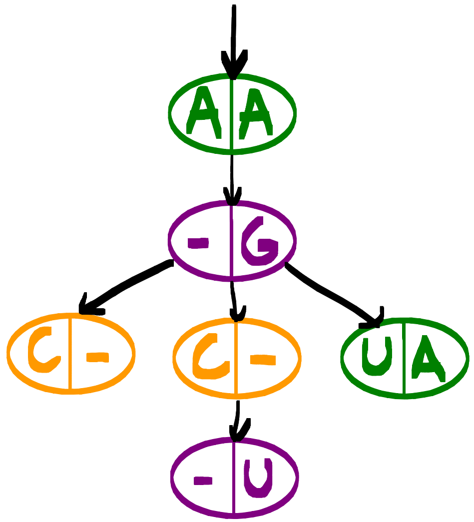


co-optimal alignments

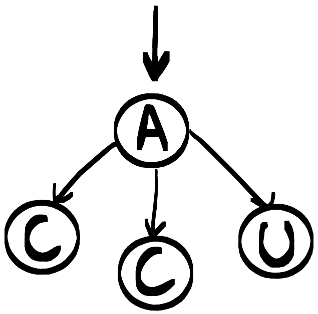
AMBIGUITY OF ALIGNMENTS

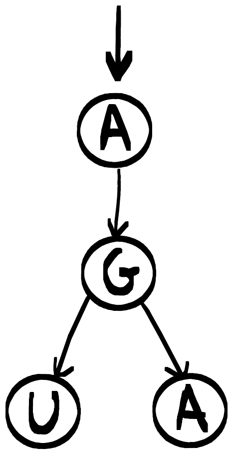
The two supertrees





induce the same alignment between the trees





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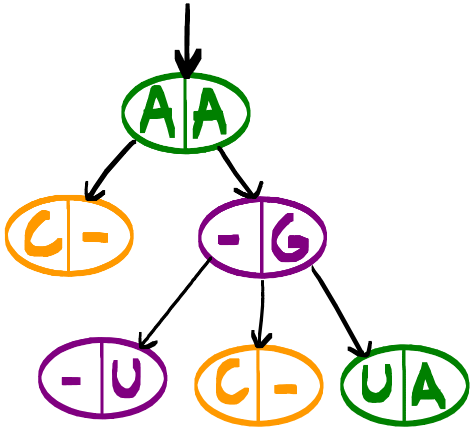
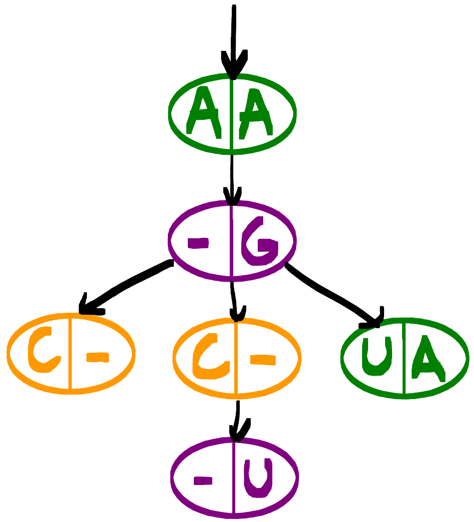
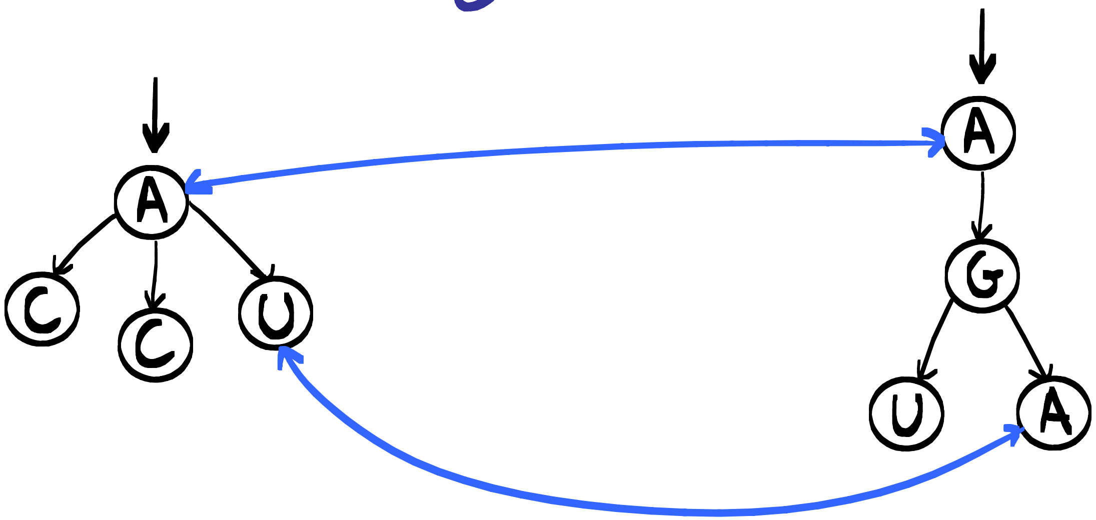




induce the same alignment between the trees



AMBIGUITY OF ALIGNMENTS

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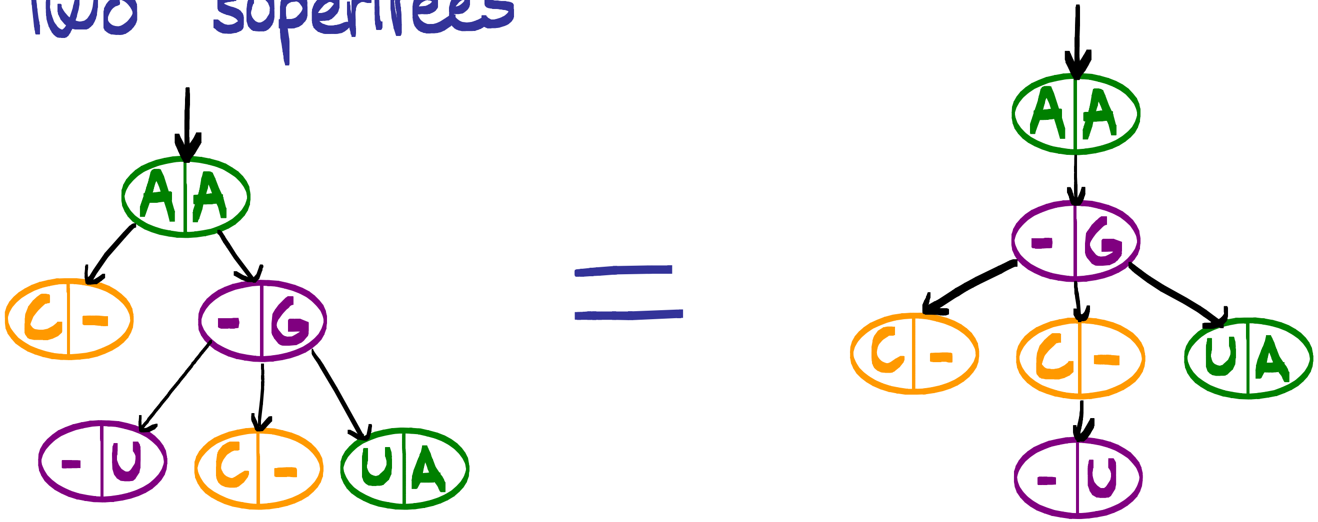

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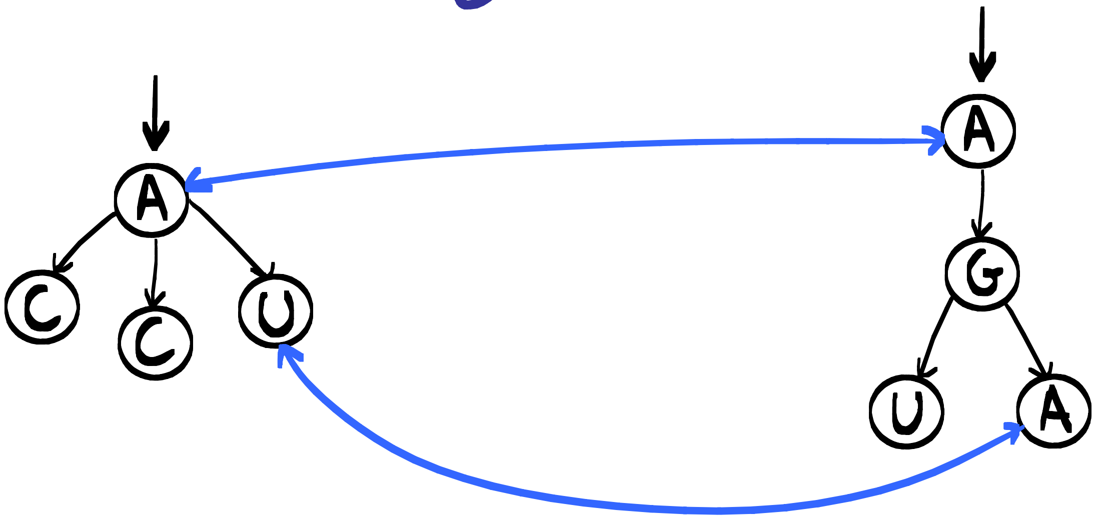

They are the same!

AMBIGUITY OF ALIGNMENTS

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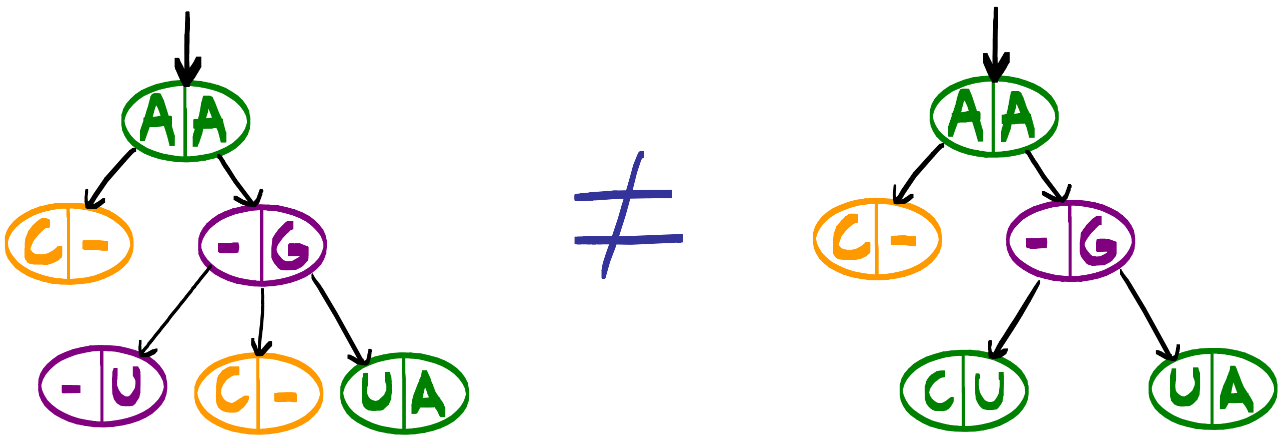
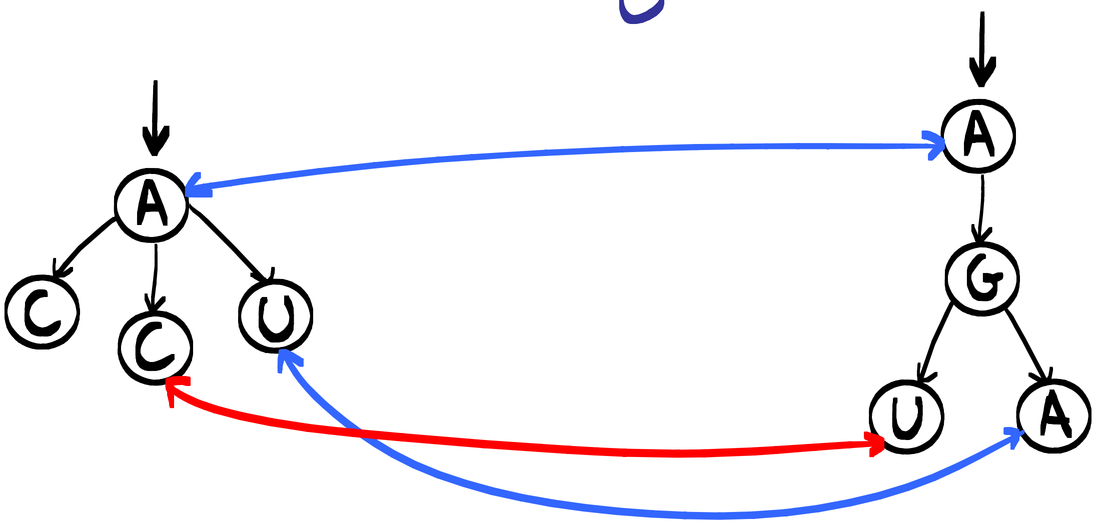


do not induce the same alignment between the trees



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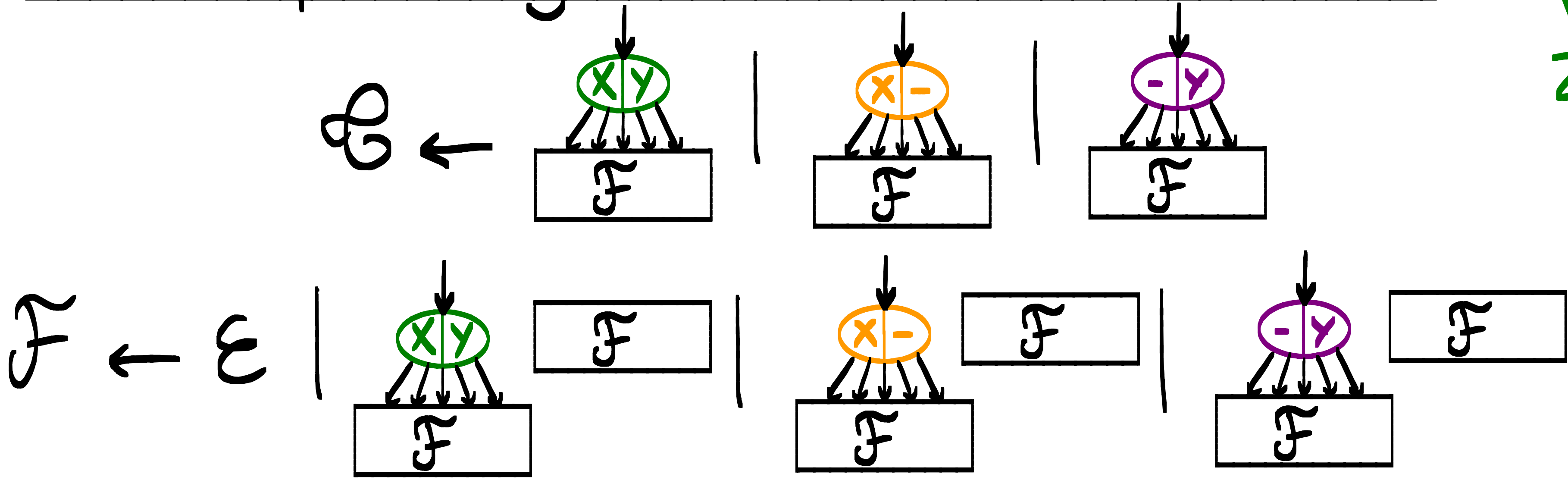

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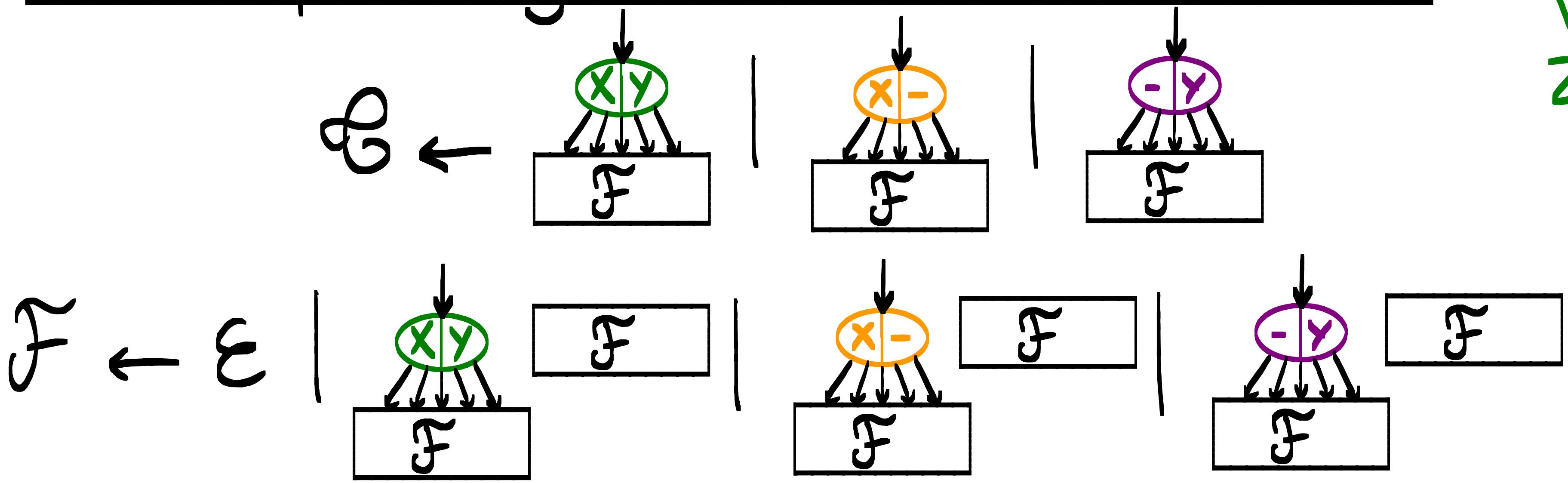

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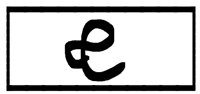

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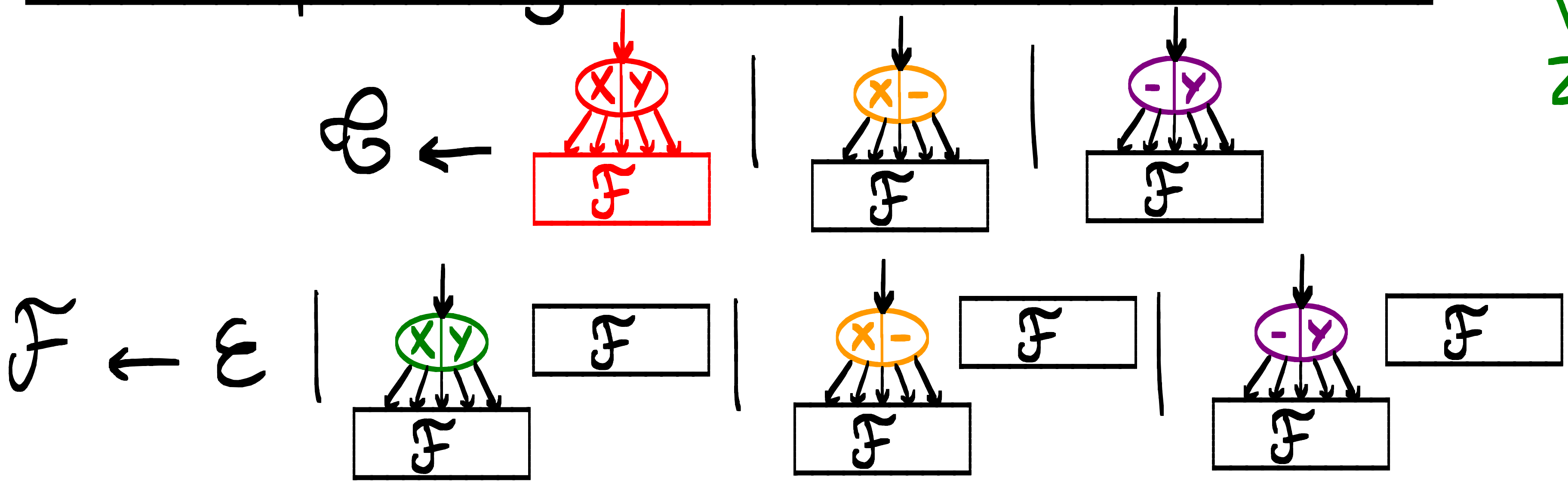

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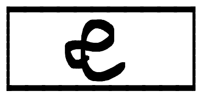

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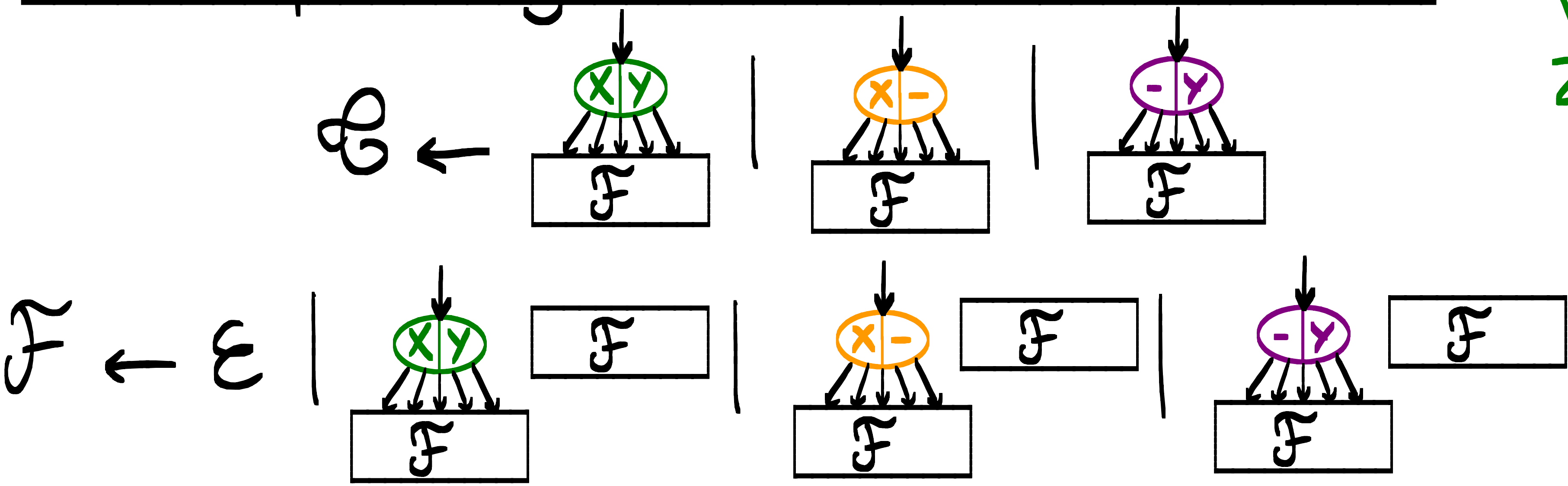

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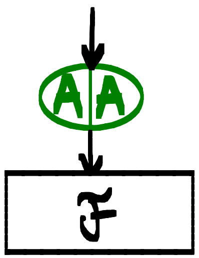

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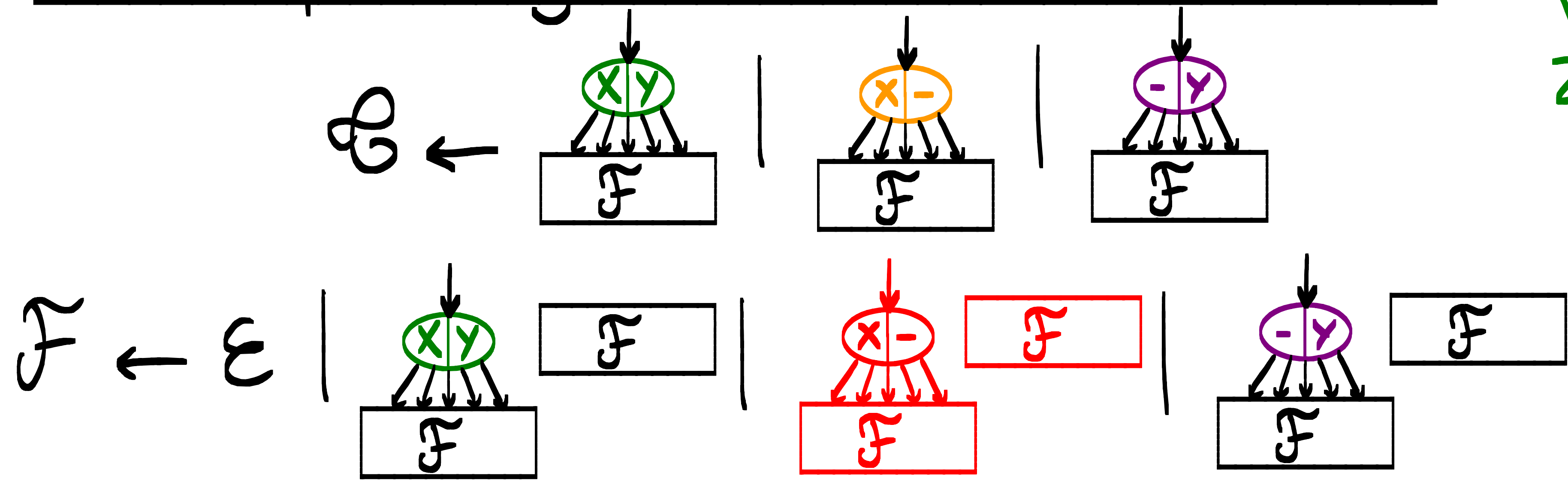

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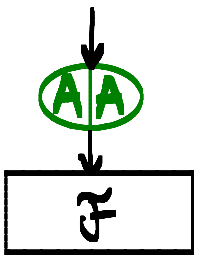

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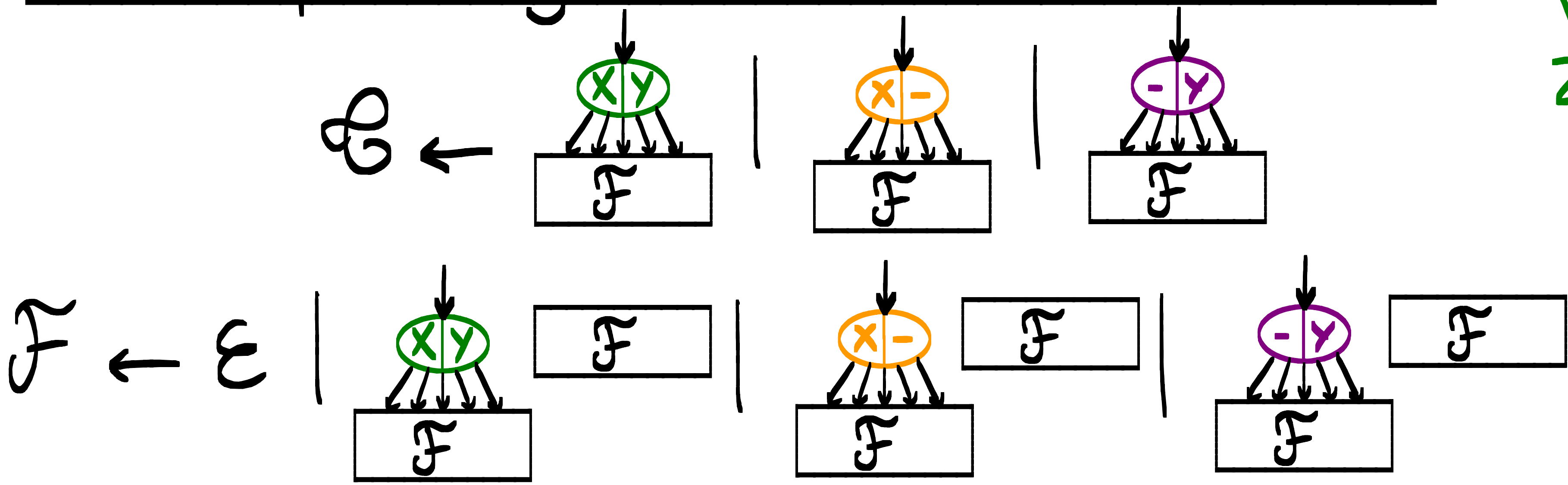

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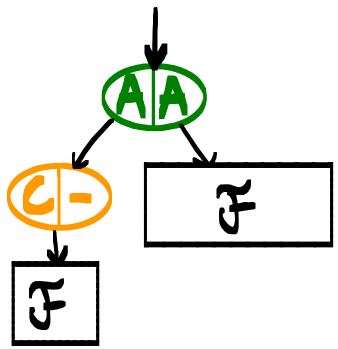

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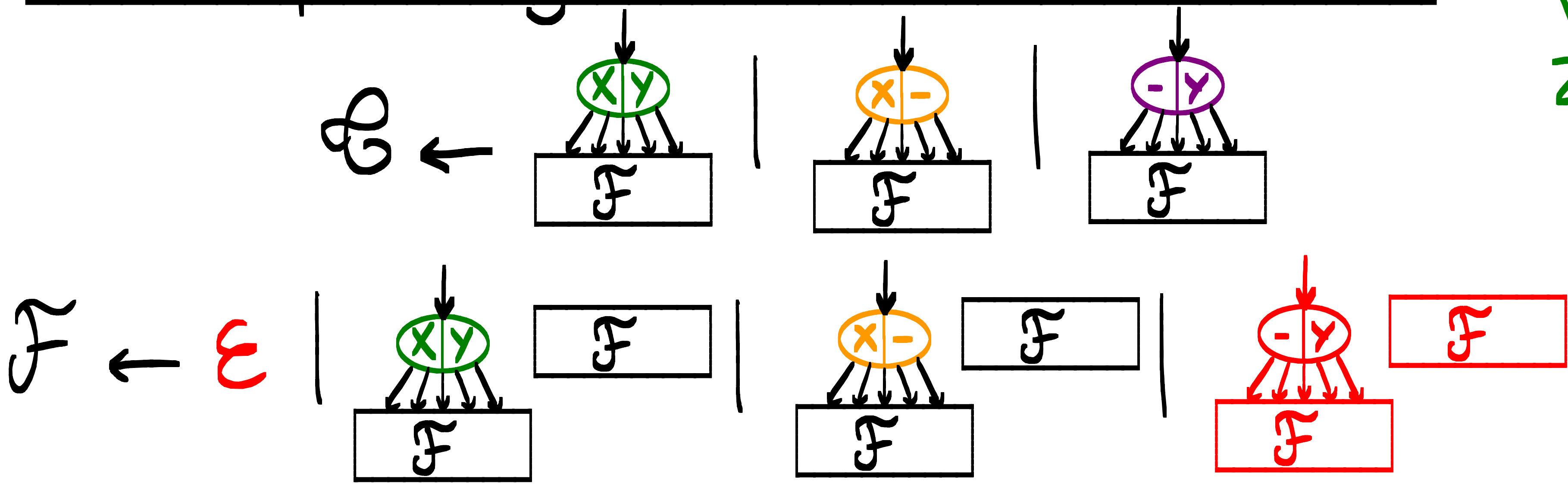

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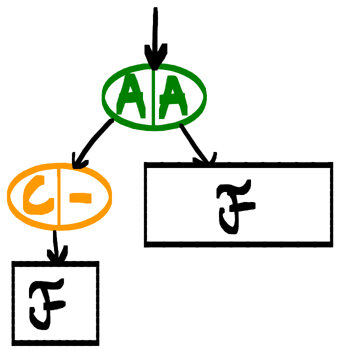

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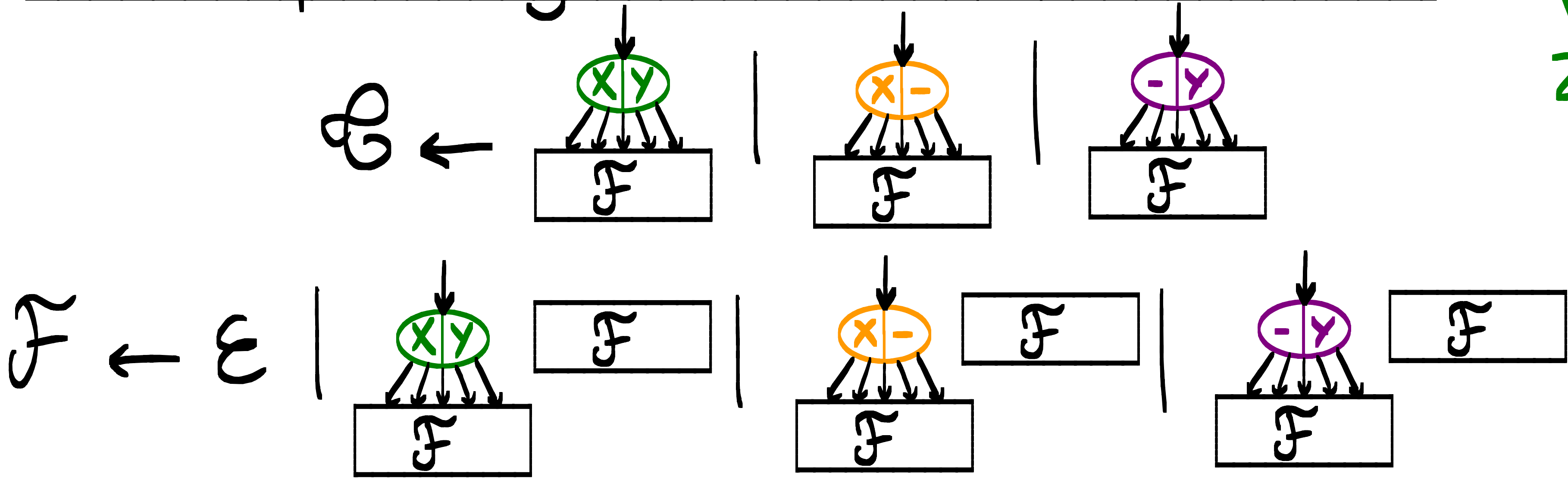

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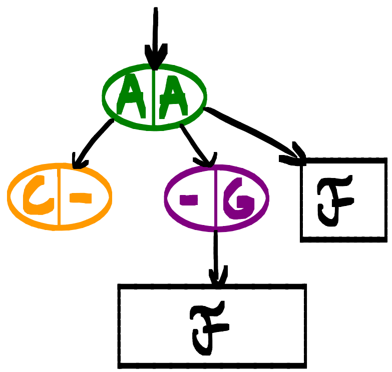

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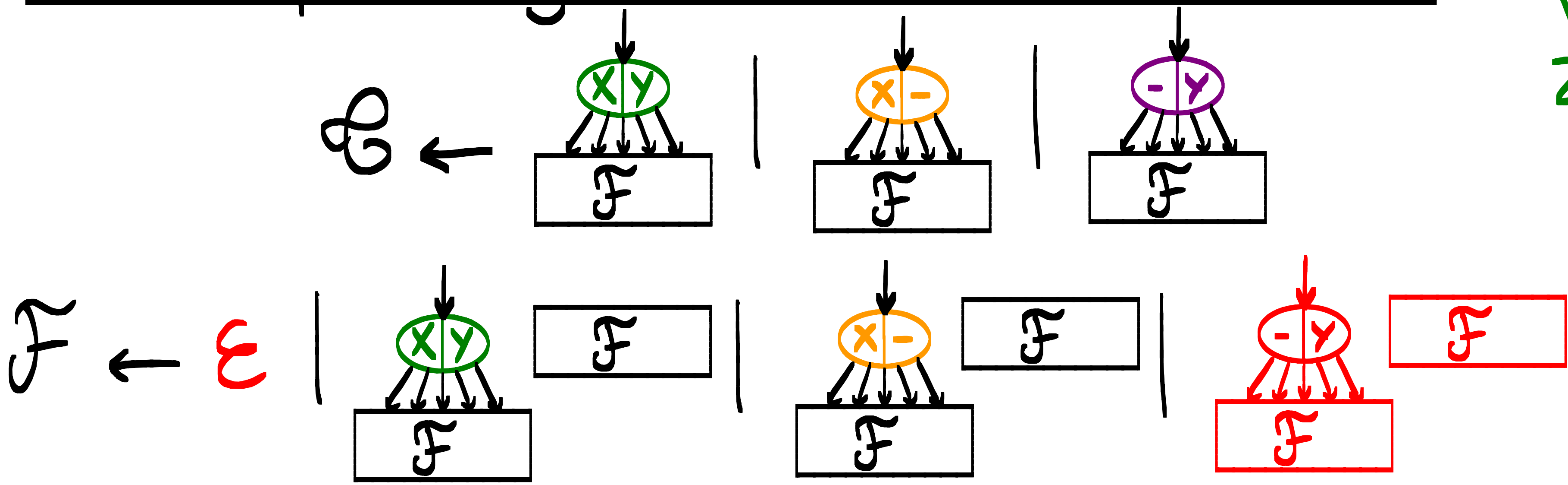

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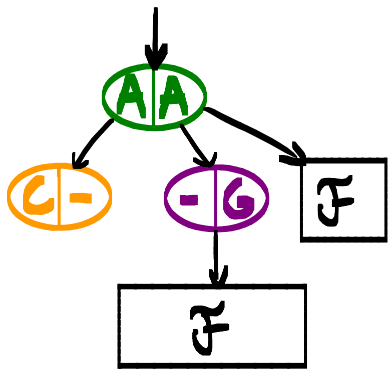

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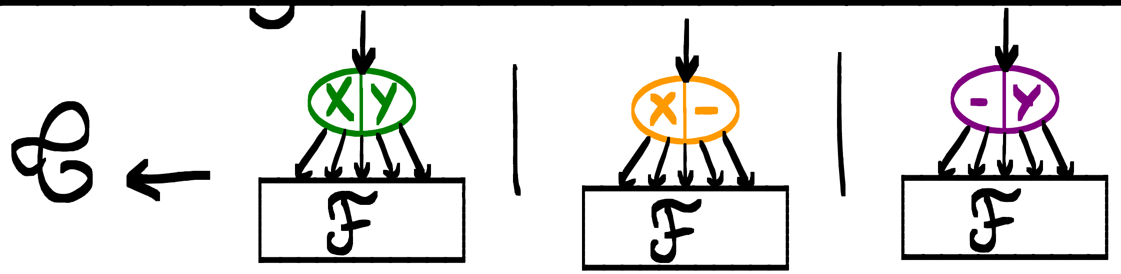

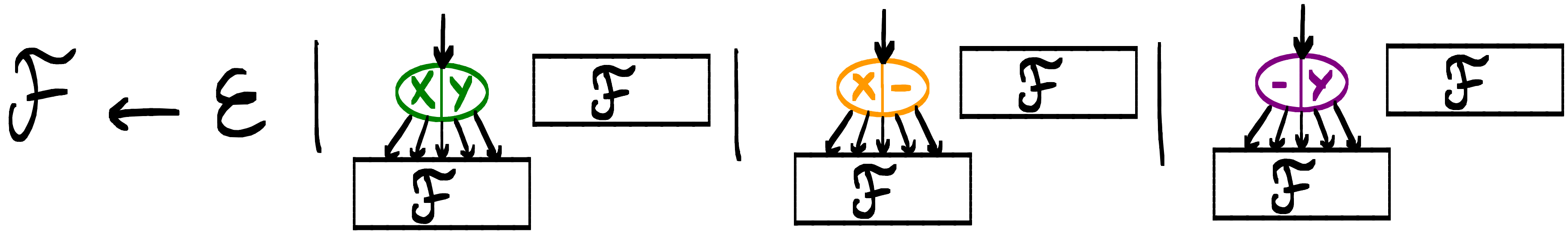

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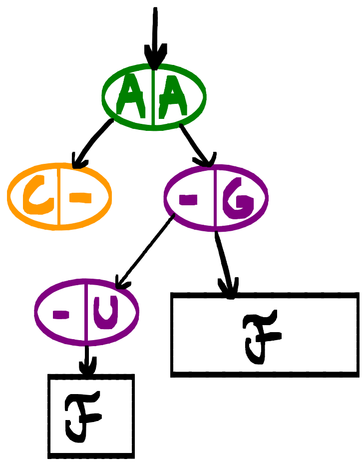

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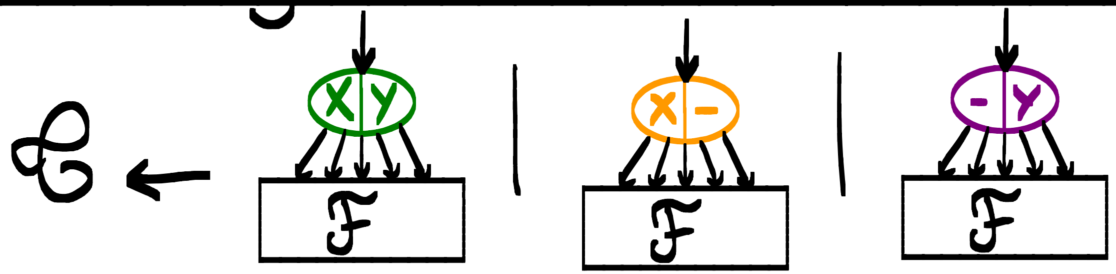

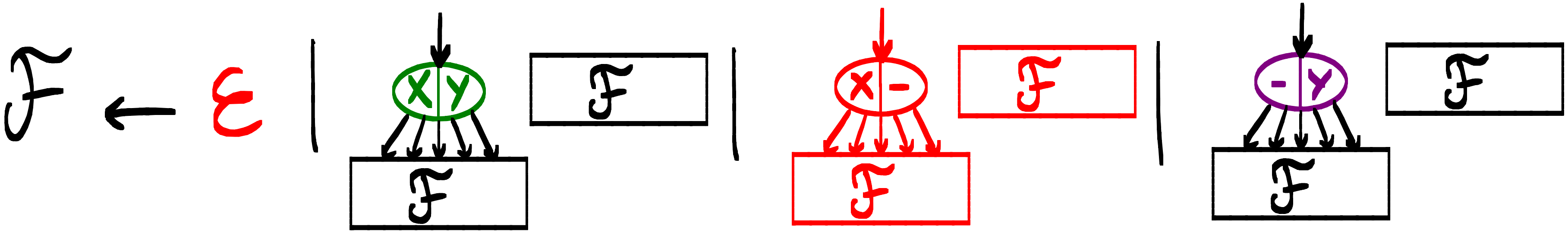

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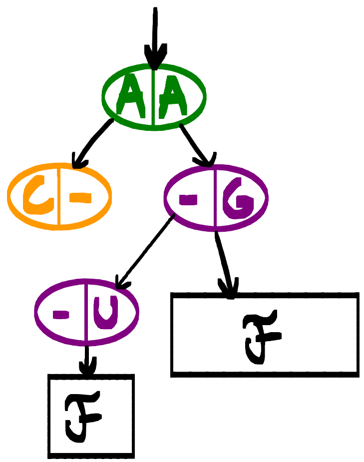

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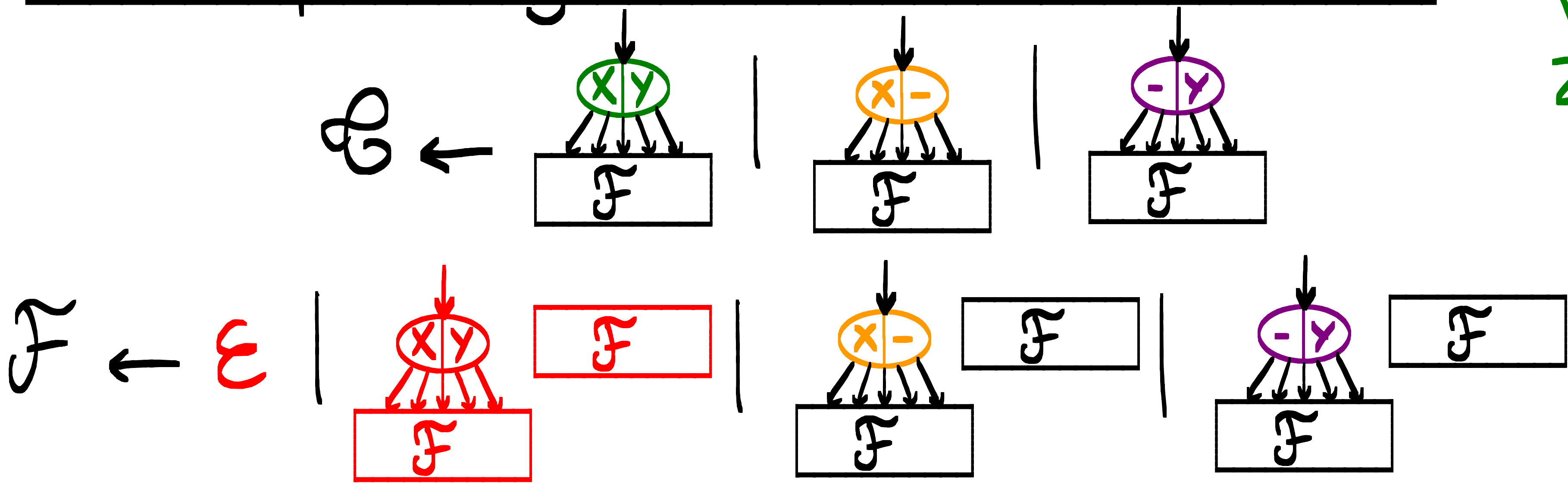

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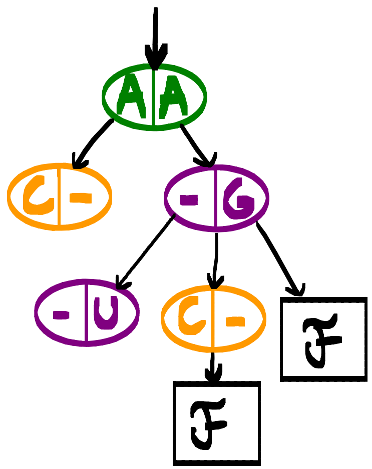

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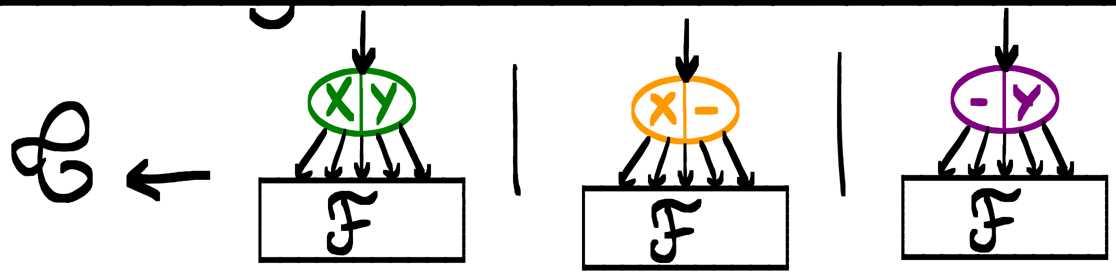

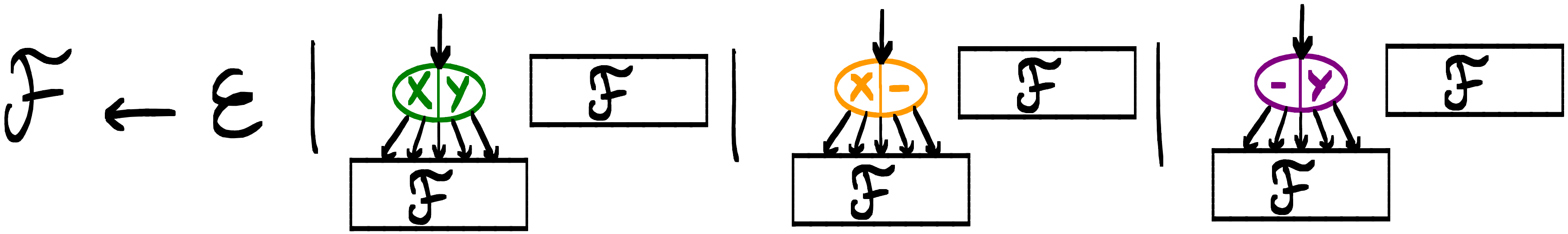

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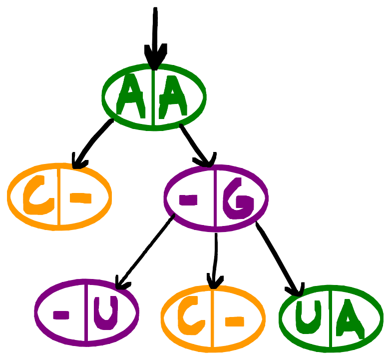

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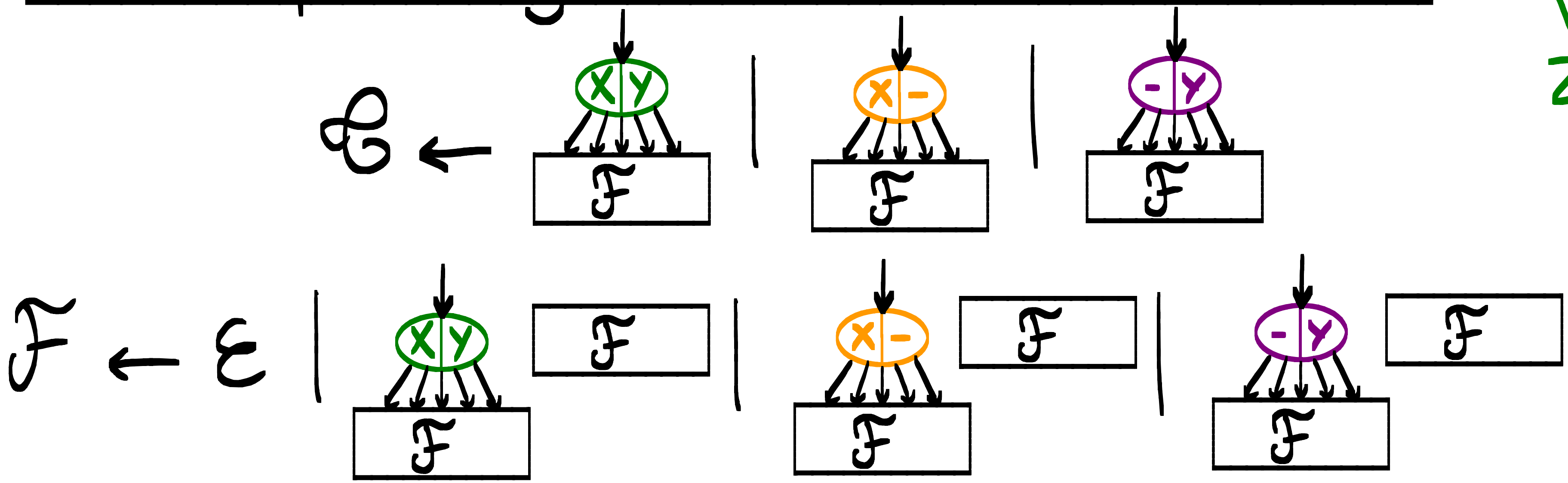

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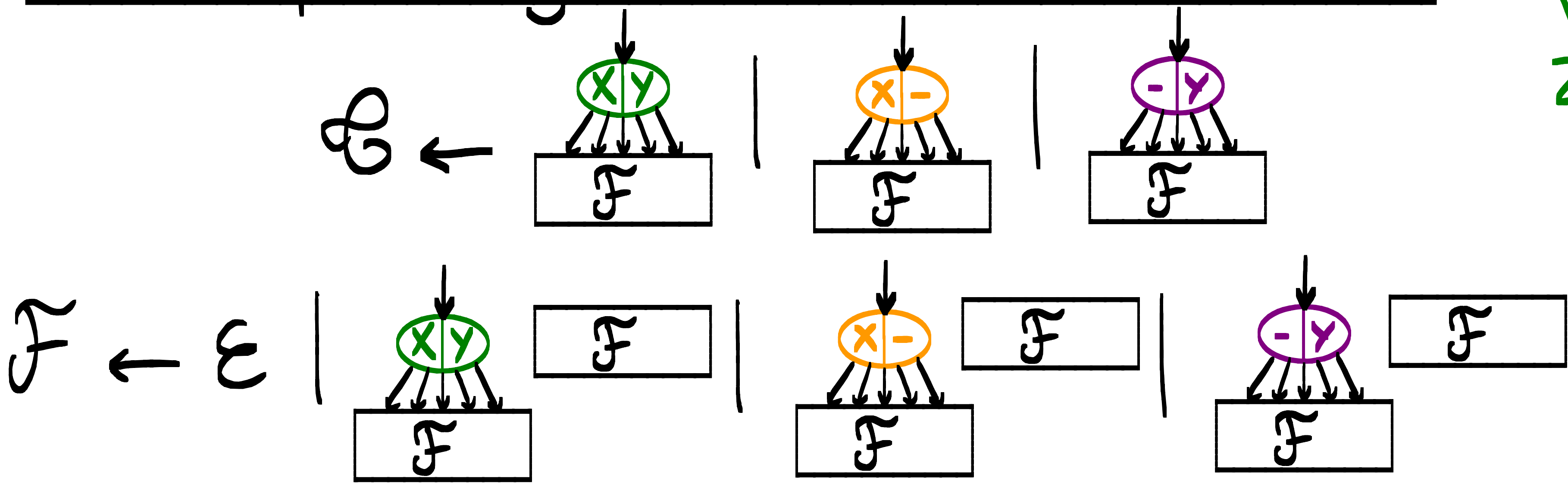

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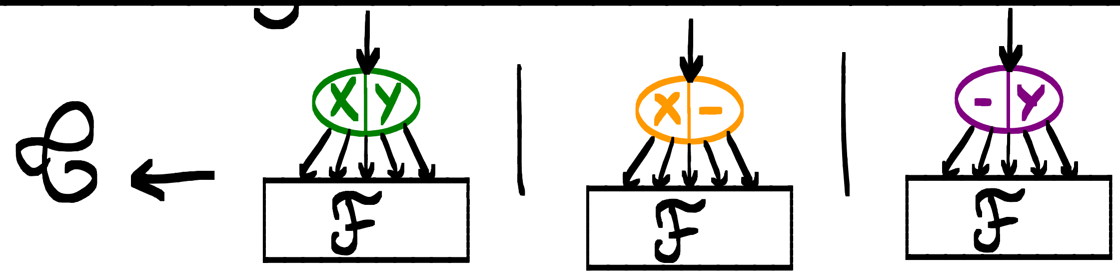

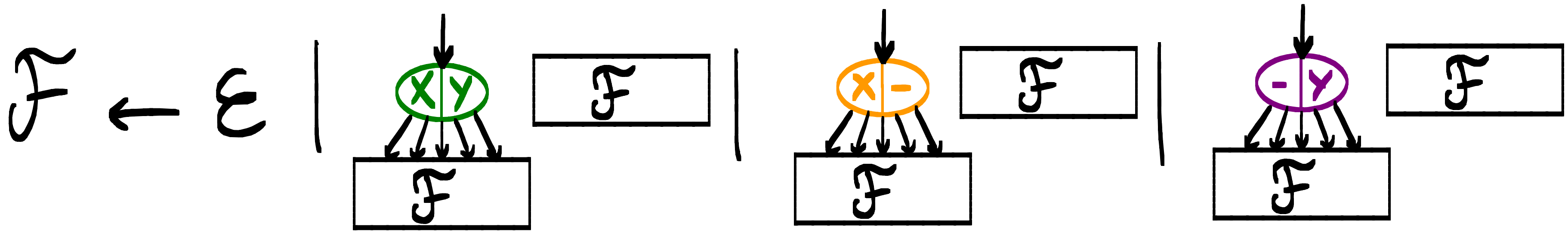

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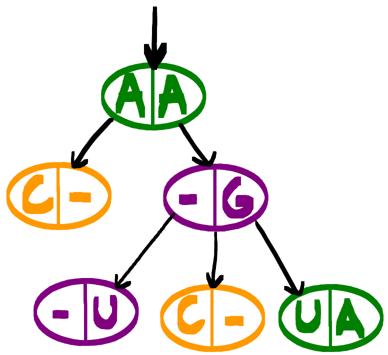

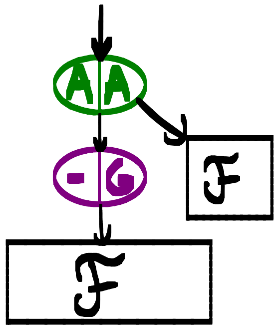

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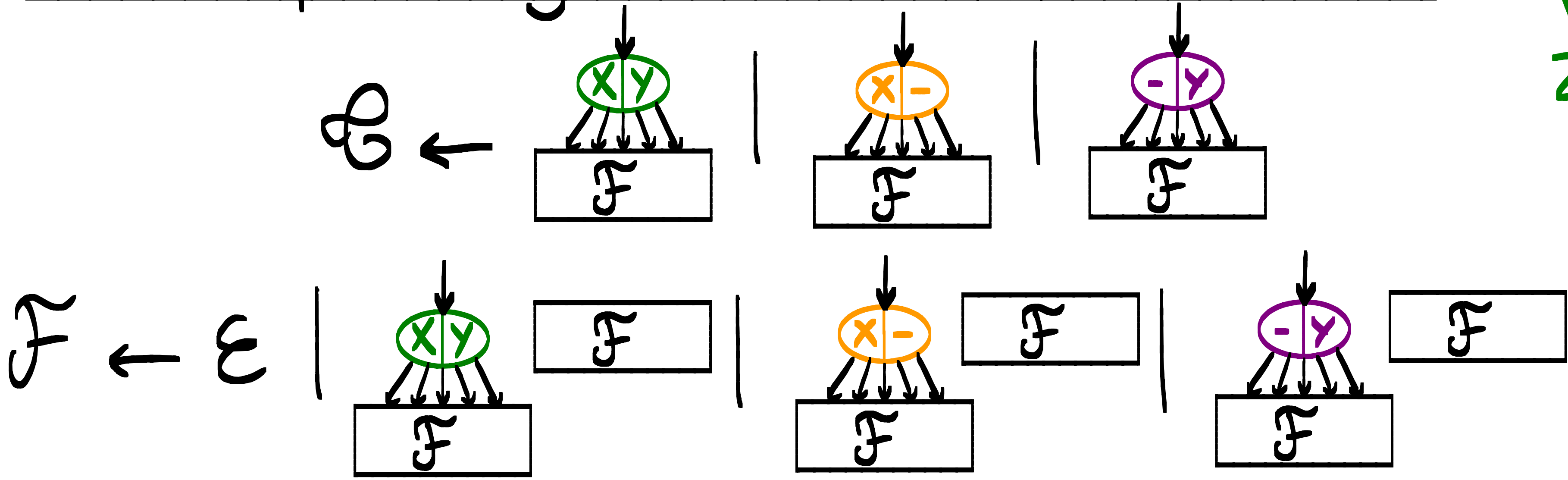

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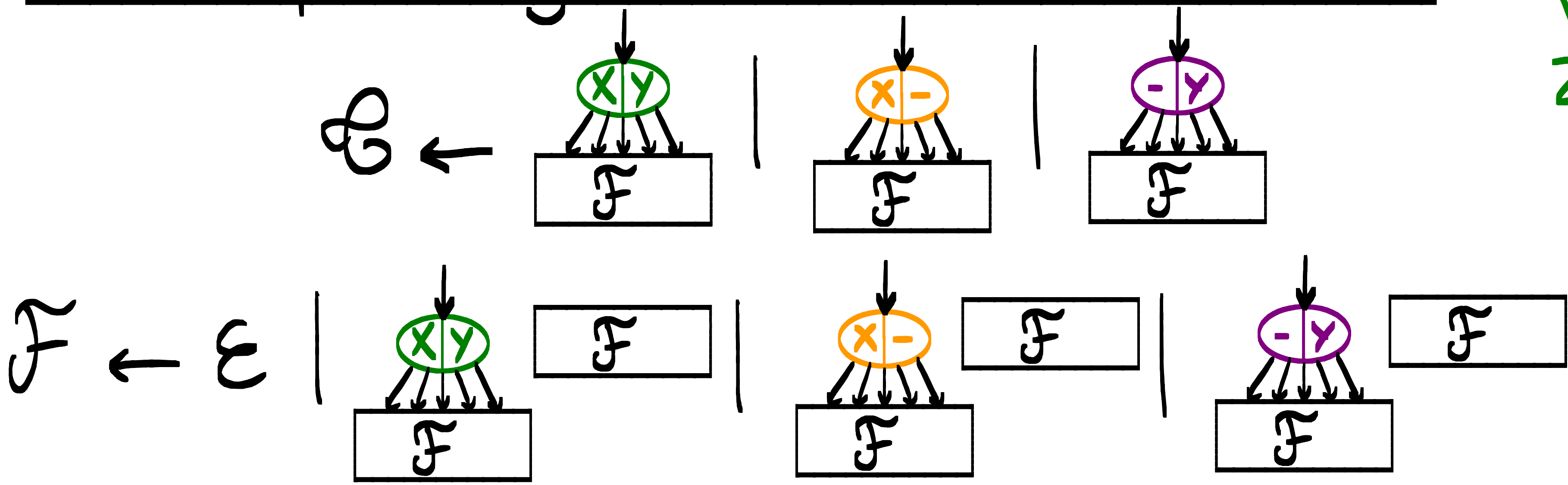

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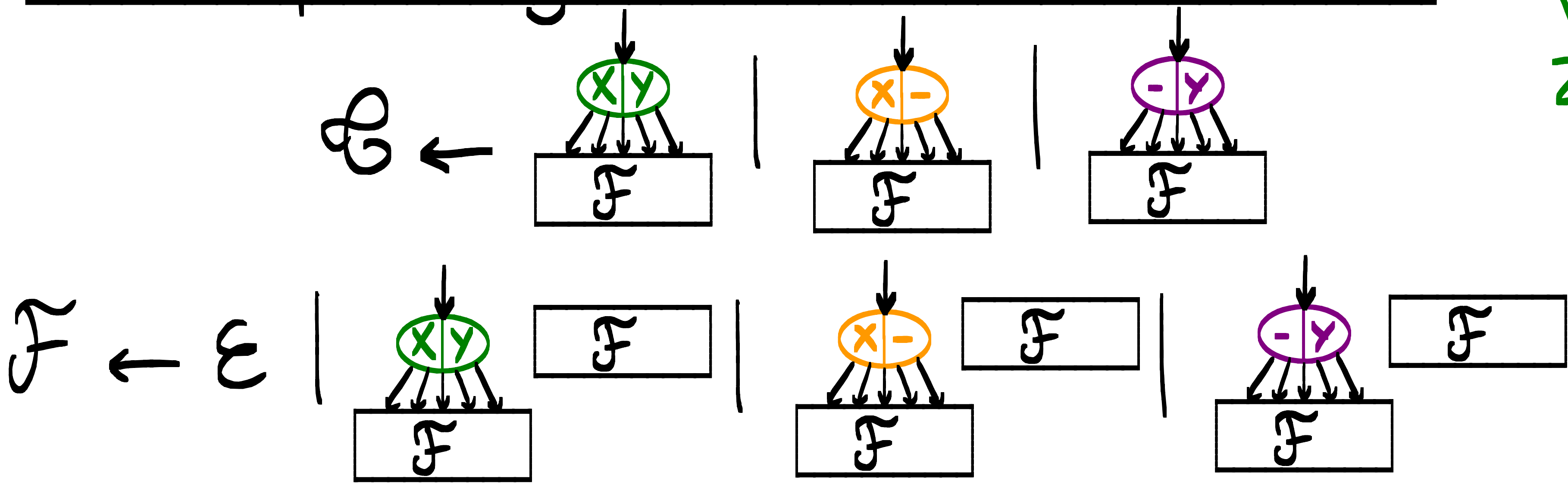

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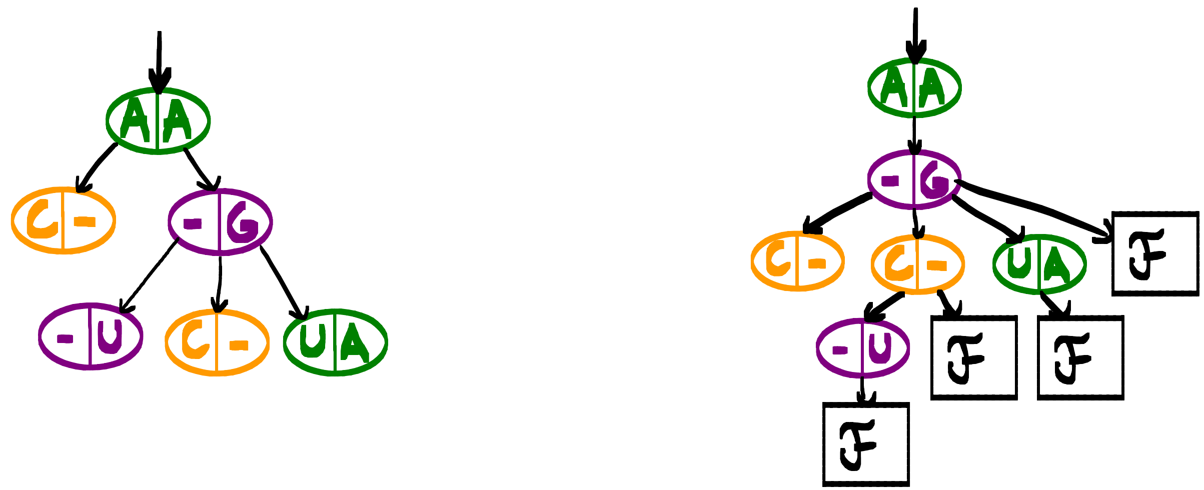

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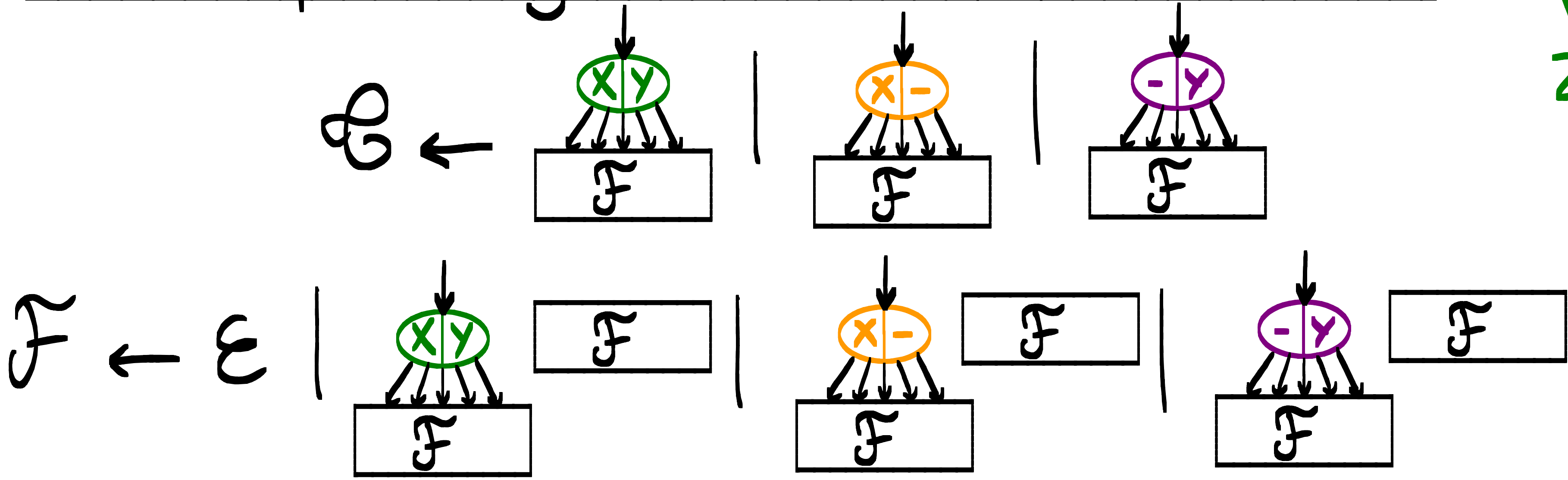

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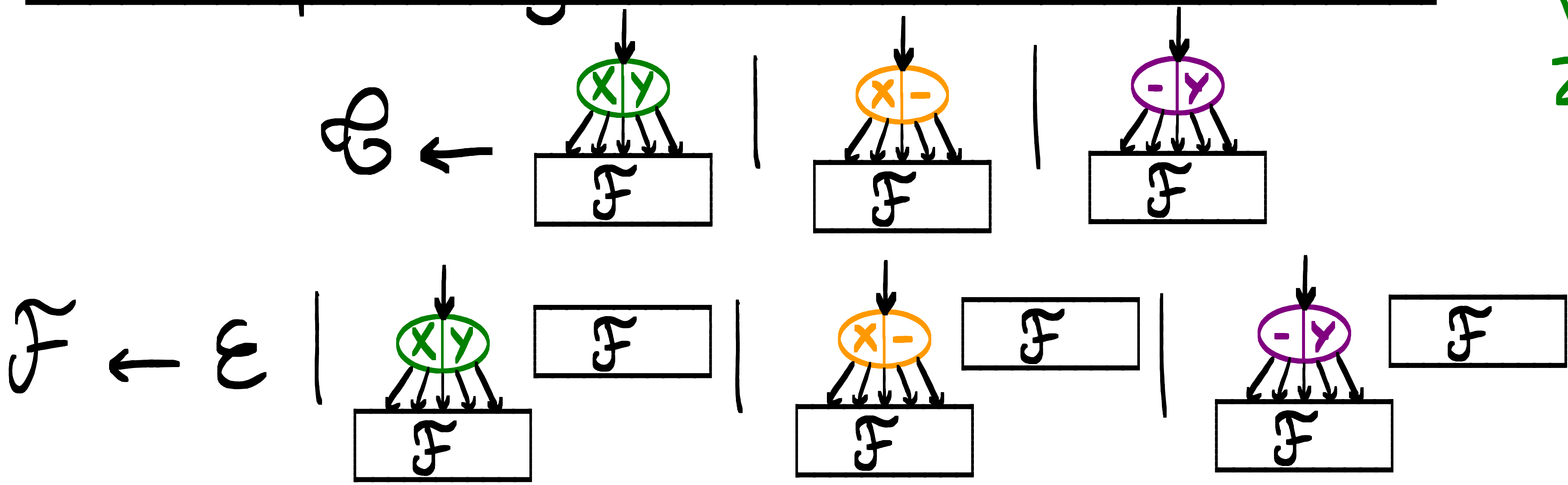

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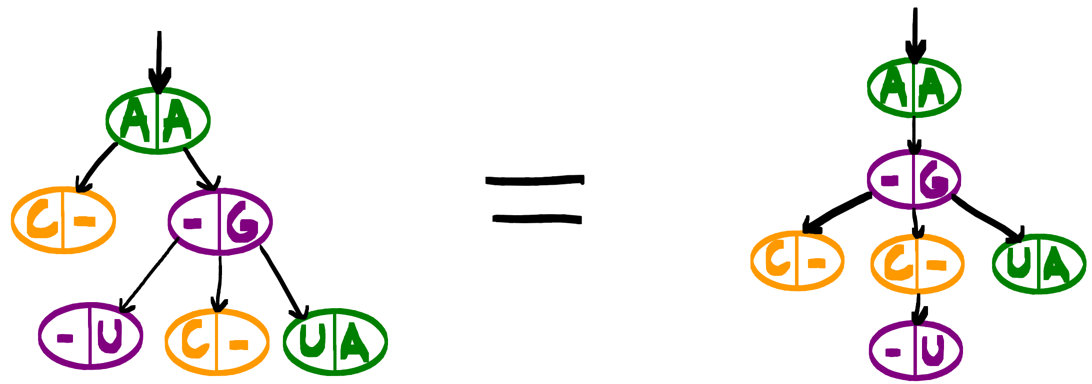


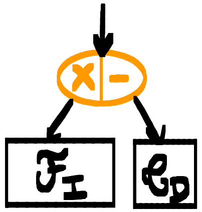
ambiguous grammar

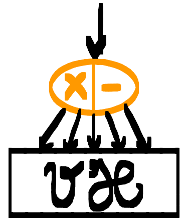
A GRAMMAR FOR ALIGNMENTS

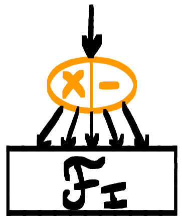
Theorem: The set of generated by the following grammar contains every tree alignment exactly once.

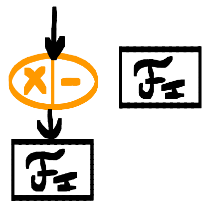
A GRAMMAR FOR ALIGNMENTS

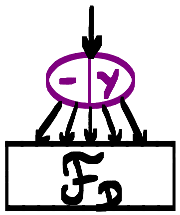
Our (complicated) non-ambiguous grammar:

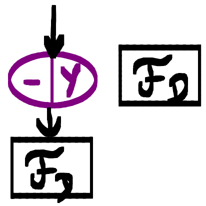
$\mathcal{A} \leftarrow \mathcal{V}^{\emptyset} \mid \mathcal{C}_I \mid \mathcal{C}_D \mid$ 

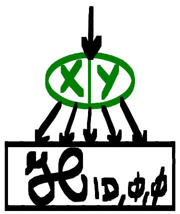
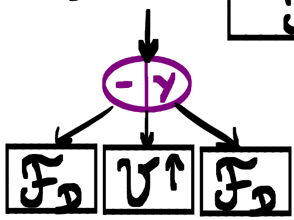
$\mathcal{V}^{\emptyset} \leftarrow \mathcal{V}^{\uparrow} \mid$ 

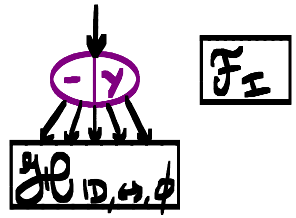
$\mathcal{C}_I \leftarrow$ 

$\mathcal{F}_I \leftarrow \varepsilon \mid$ 

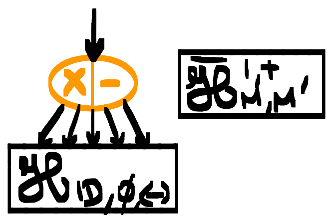
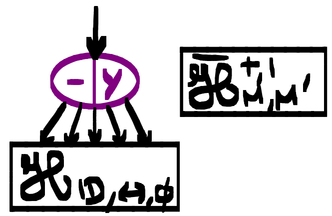
$\mathcal{C}_D \leftarrow$ 

$\mathcal{F}_D \leftarrow \varepsilon \mid$ 

$\mathcal{V}^{\uparrow} \leftarrow$  $\mid$ 

$\mathcal{VH} \leftarrow \boxed{\mathcal{F}_I}\boxed{\mathcal{VH}} \mid \boxed{\mathcal{V}^{\emptyset}}\boxed{\mathcal{F}_I} \mid$ 

For $\mathcal{V} \in \{\mathbb{D}, \mathcal{D}\}$, $(M, M') \in \{\emptyset, \rightarrow, \leftrightarrow\}^2$:

$\mathcal{B}_{\mathcal{V},M,M'} \leftarrow \varepsilon \mid \boxed{\mathcal{C}_I}\boxed{\mathcal{B}_{\mathcal{V},M,M'}} \mid \boxed{\mathcal{C}_D}\boxed{\mathcal{B}_{\mathcal{D},M,M'}} \mid \boxed{\mathcal{V}^{\emptyset}}\boxed{\overline{\mathcal{B}}_{M,M'}} \mid$  $\mid$ 

only if $(M,M') = (\emptyset,\emptyset)$

only if $\mathcal{V} \neq \mathcal{D}$ and $M \neq \leftrightarrow$

only if $M' \neq \leftrightarrow$

no room for $\overline{\mathcal{B}}^{i,j}_{M,M'}$...

APPLICATION 1: COUNTING.

a_n = number of tree alignments of size n

Generating function: $A(z) = \sum_{n \geq 0} a_n z^n$

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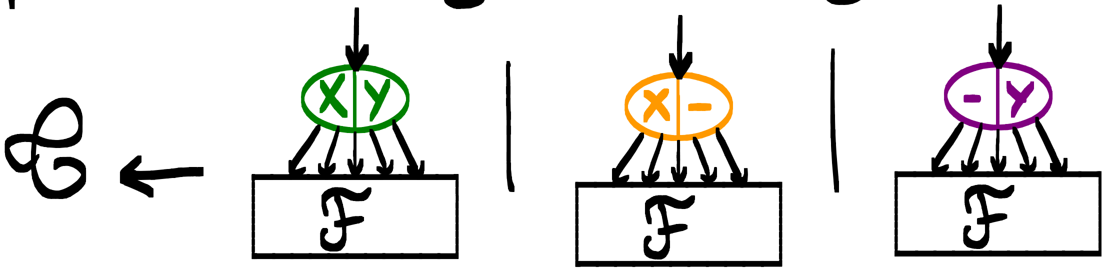
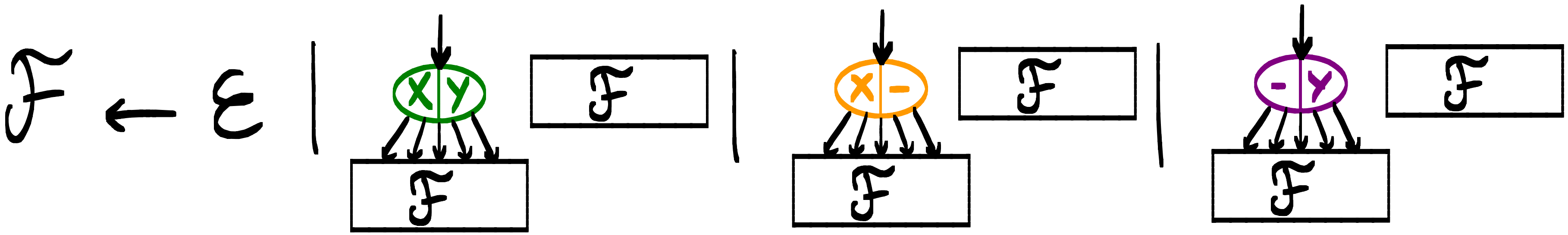
The principle on Jiang et al.'s grammar:





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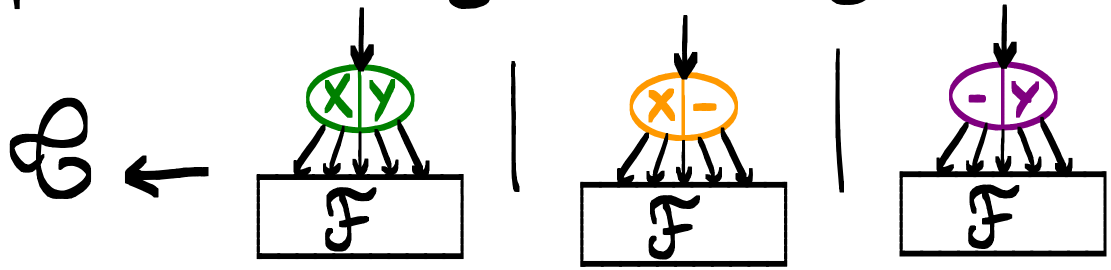
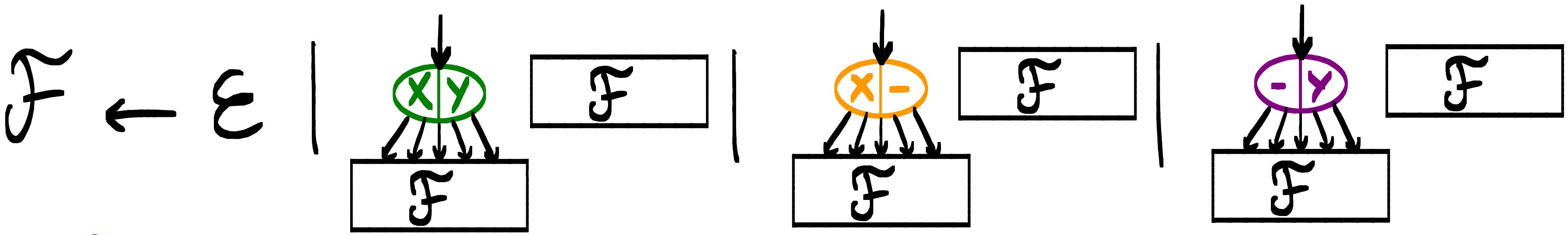


$$T(z) = F(z) + F(z) + F(z)$$



$$F(z) = 1 + F(z) \times F(z) + F(z) \times F(z) + F(z) \times F(z)$$

APPLICATION 1: COUNTING.

a_n = number of tree alignments of size n

Generating function: $A(z) = \sum_{n \geq 0} a_n z^n$

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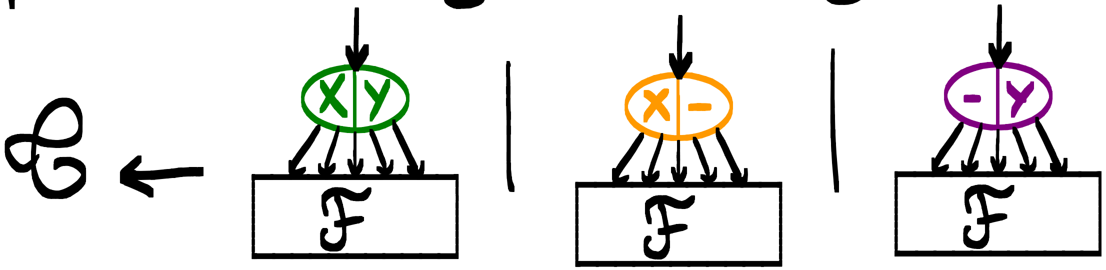

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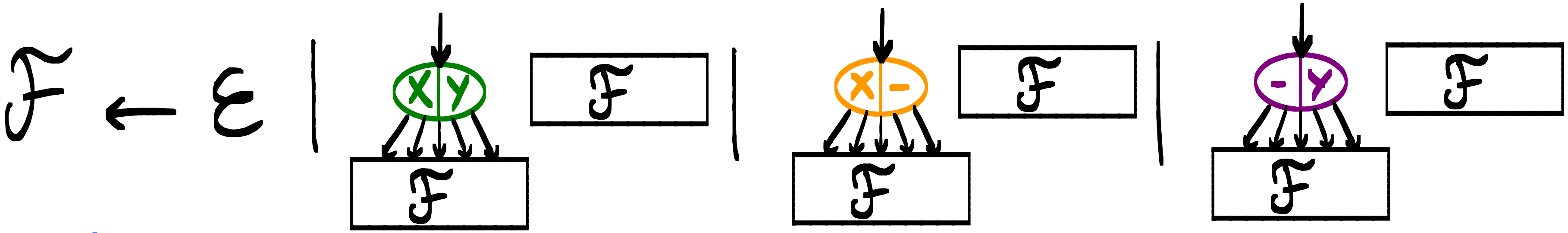

$$F(z) = 1 + F(z)^2 + F(z)^2 + F(z)^2$$

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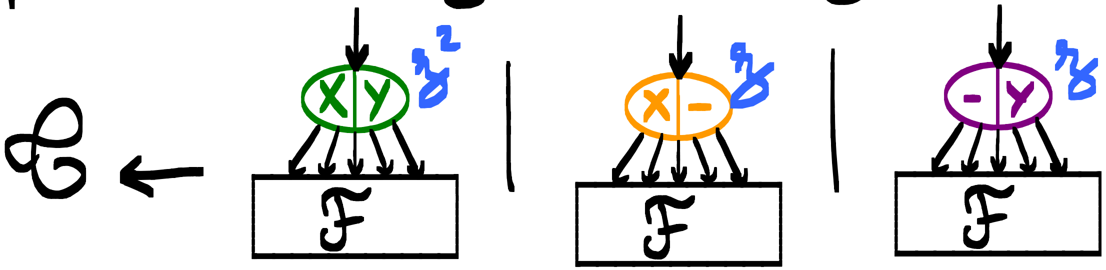

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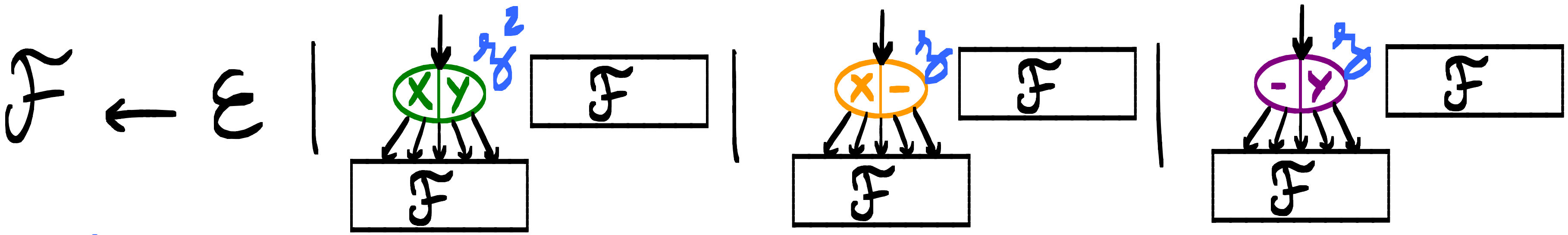

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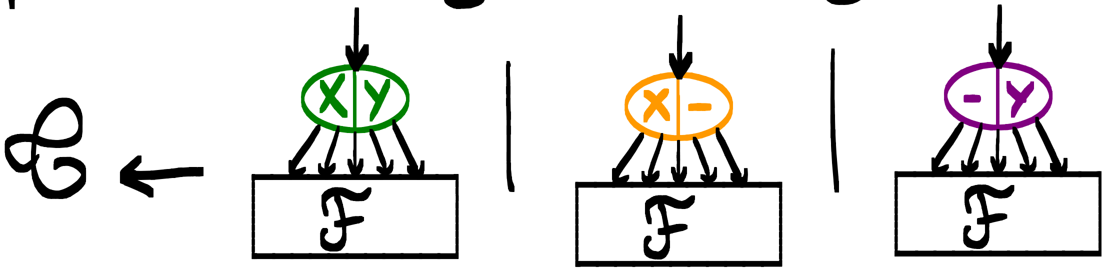
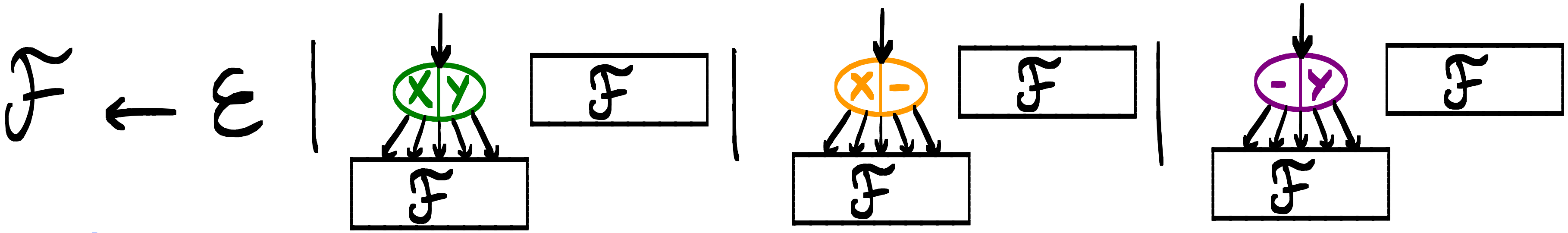


$T(z) = z^2 \times F(z) + z \times F(z) + z \times F(z)$



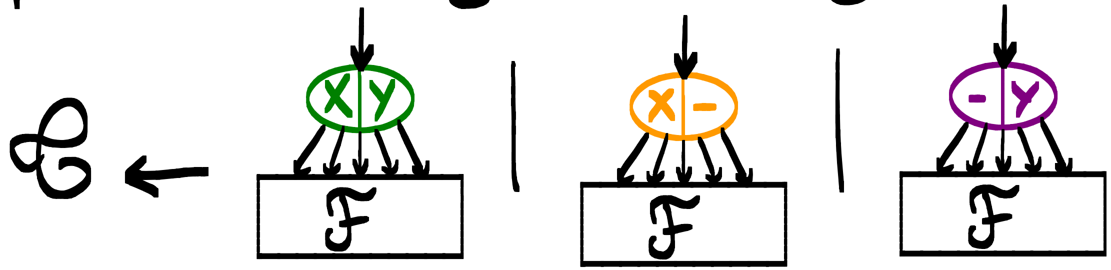
$F(z) = 1 + z^2 \times F(z)^2 + z \times F(z)^2 + z \times F(z)^2$

APPLICATION 1: COUNTING.

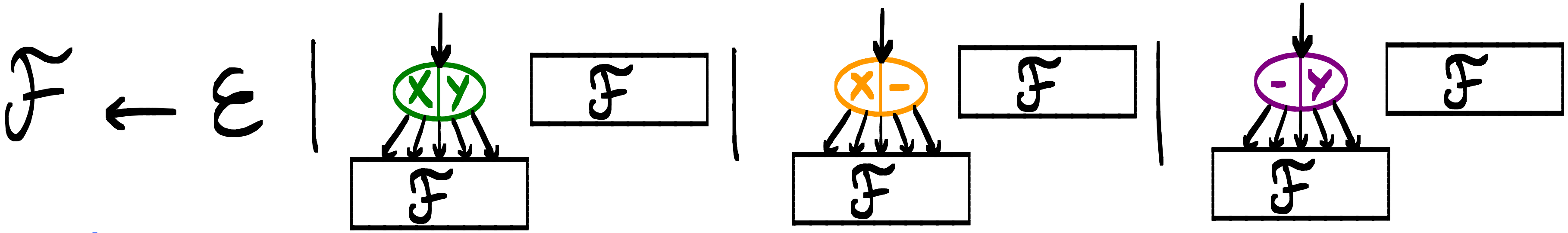
$a_{n,k}$ = number of tree alignments of size n and k matches

Generating function: $A(z,u) = \sum_{n \geq 0} a_{n,k}\, z^n u^k$

The principle on Jiang et al.'s grammar:



$$T(z,u) = u \times z^2 F(z,u) + z \times F(z,u) + z \times F(z,u)$$



$$F(z,u) = 1 + u \times z^2 \times F(z,u)^2 + z \times F(z,u)^2 + z \times F(z,u)^2$$

APPLICATION 1: COUNTING.

Theorem: The generating function $A(z,u)$ of tree alignments satisfies

$$A(z,u) = \left(z^2 + z - uz^2 + \frac{z}{\sqrt{1-4z}}\right) \times B(z,u)$$

where

$$\left(uzC(z)^2 - z^2C(z)^2 + 2z\right)B(z,u)^2 + \left(z^2C^4(z) - 2zC(z)^2 - 1\right)B(z,u) + C^2(z) = 0$$

and

$$C(z) = \frac{1-\sqrt{1-4z}}{2z}$$ Catalan generating function

SOME STATISTICAL PROPERTIES

<u>Theorem</u> There are on average

$C \times 1.5^n$ alignments

between two random trees of cumulative size n

where $C = 0.299\ldots$

<u>Corollary</u>: A same alignment was repeated

$\sim 0.875 \times 1.412^n$ times on

average in the previous

ambiguous grammar.

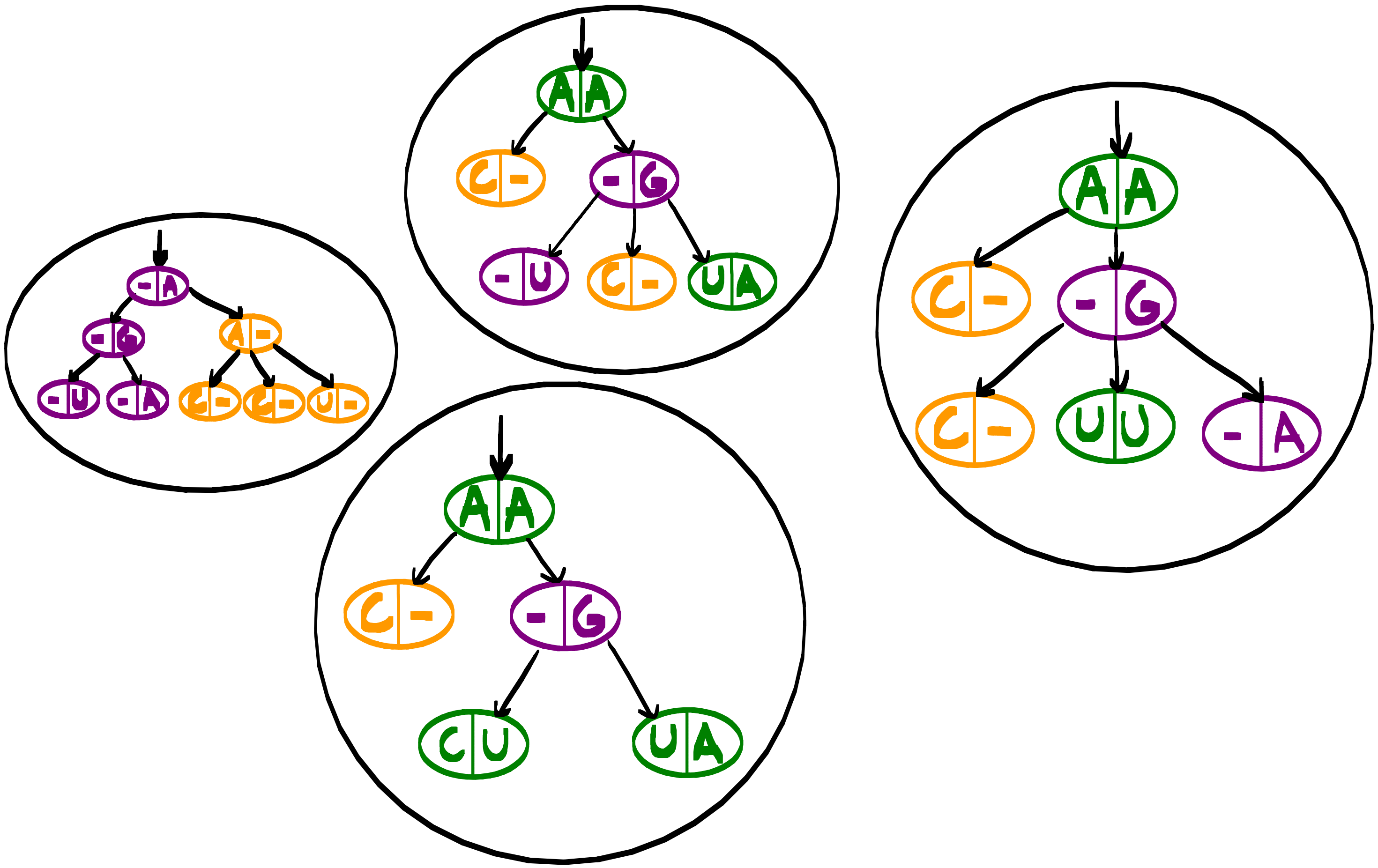
APPLICATION 2 - SAMPLING

Objective: Sampling alignments under the Gibbs-Boltzmann probability distribution.

probability of an alignment A

$$\propto e^{-\frac{cost(A)}{K}}$$

(Gibbs-Boltzmann distribution)



APPLICATION 2. SAMPLING

Objective: Sampling alignments under the Gibbs-Boltzmann probability distribution.

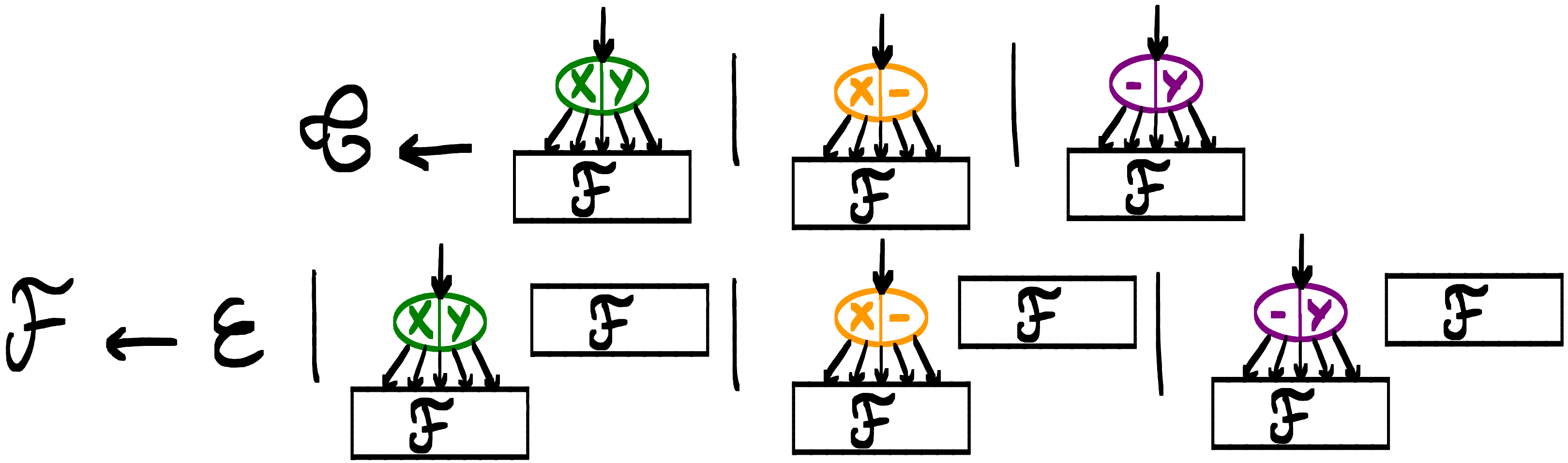
Strategy:

→ Filter the grammar to obtain a new grammar that only generates alignments between two fixed trees S and T

→ Use dynamic programming.

GRAMMAR OF ALIGNMENTS BETWEEN TWO FIXED TREES

The principle on Jiang et al.'s grammar:



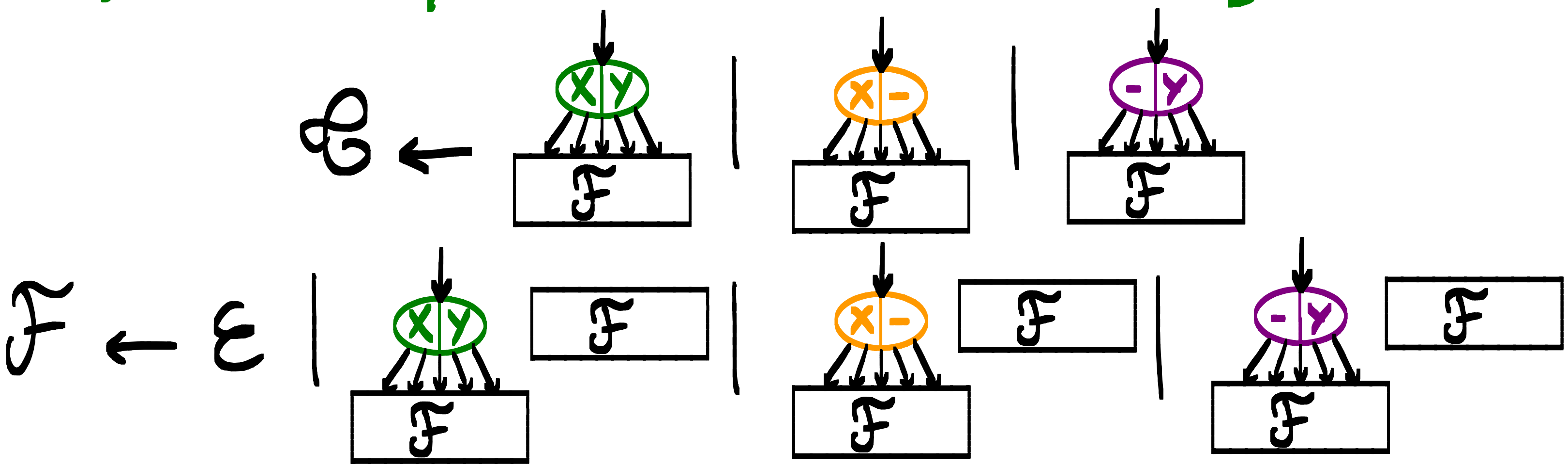
GRAMMAR OF ALIGNMENTS BETWEEN TWO FIXED TREES

The principle on Jiang et al.'s grammar:

We fix two trees S and T.

Let F be a subforest of S and G a subforest of T

$J[F,G] = \{\text{alignments between } F \text{ and } G\}$



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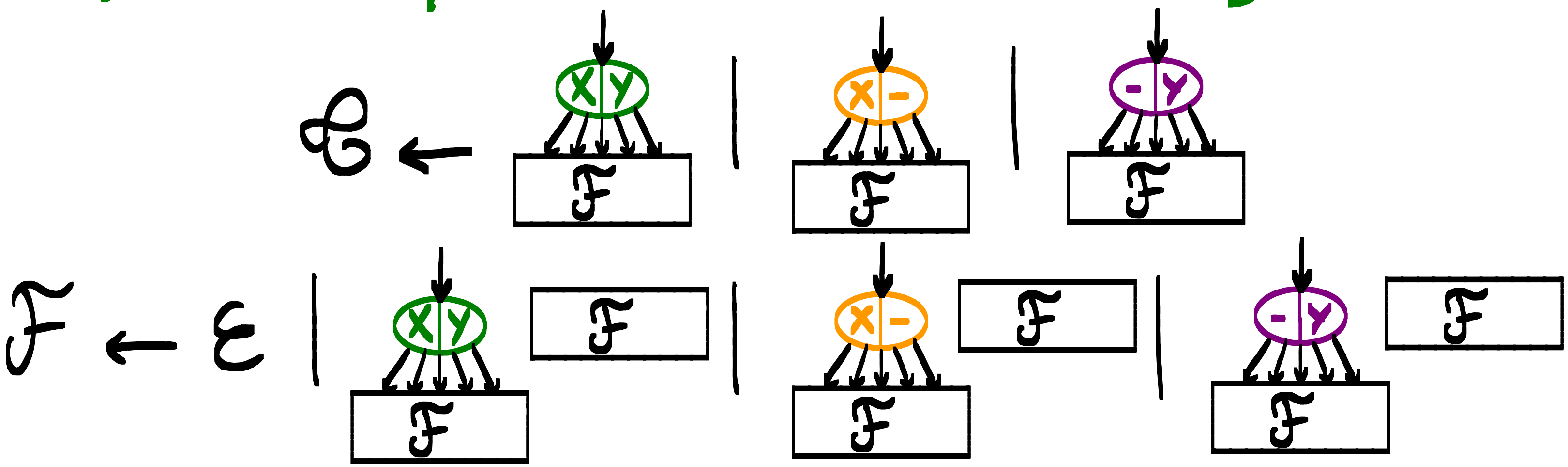

If $F = \emptyset$ and $G = \emptyset$, then

$$J[F,G] \leftarrow \varepsilon$$

GRAMMAR OF ALIGNMENTS BETWEEN TWO FIXED TREES

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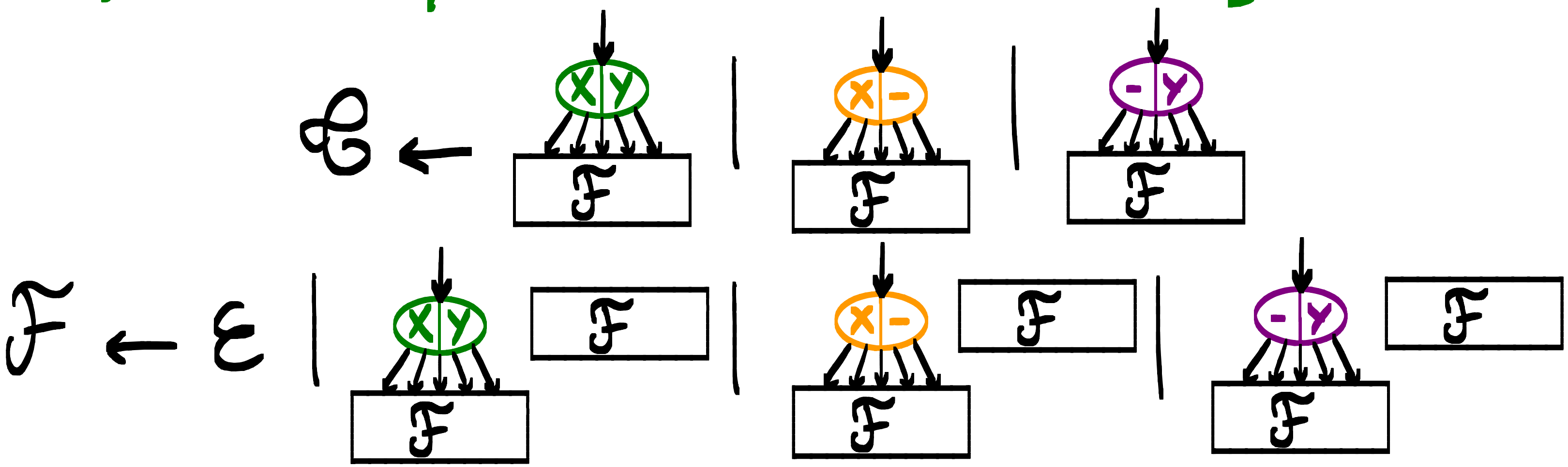
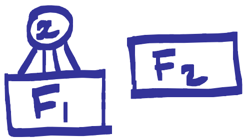
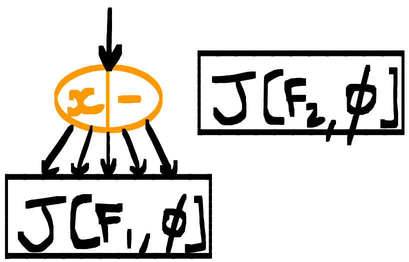


If $F =$  and $G = \emptyset$, then

$J[F,G] \leftarrow$ 

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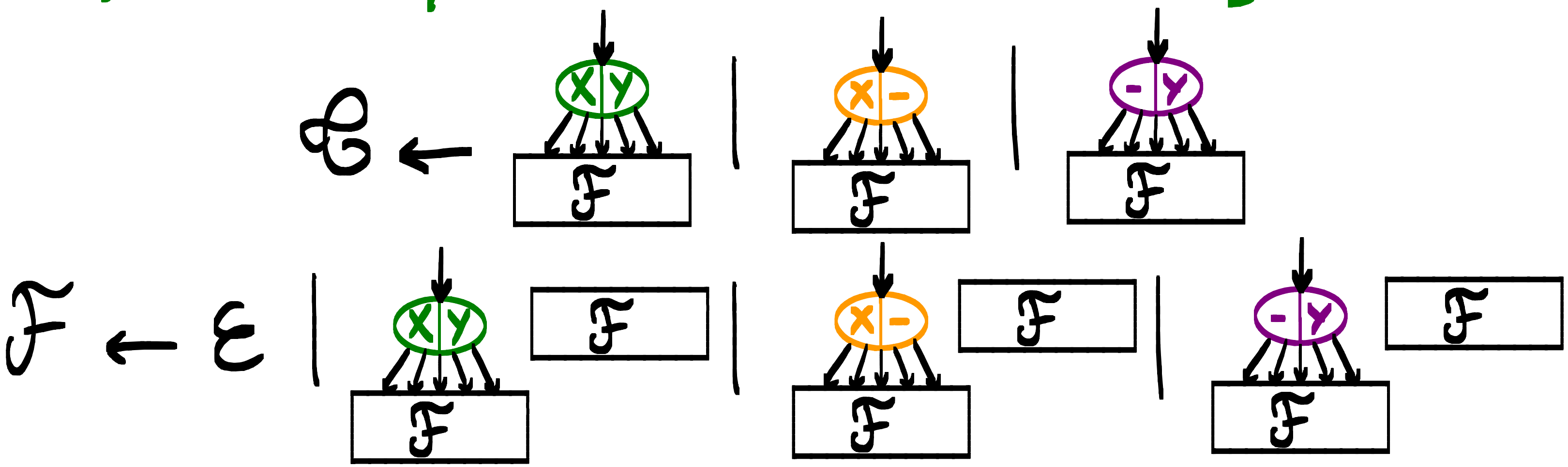
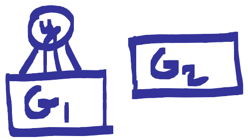


If $F = \emptyset$ and $G =$ 

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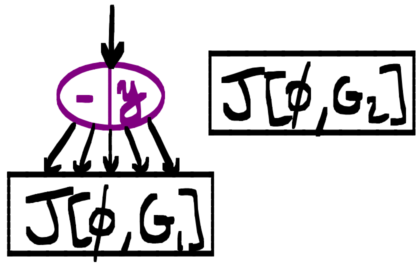
$J[F,G] \leftarrow$ 

GRAMMAR OF ALIGNMENTS BETWEEN TWO FIXED TREES

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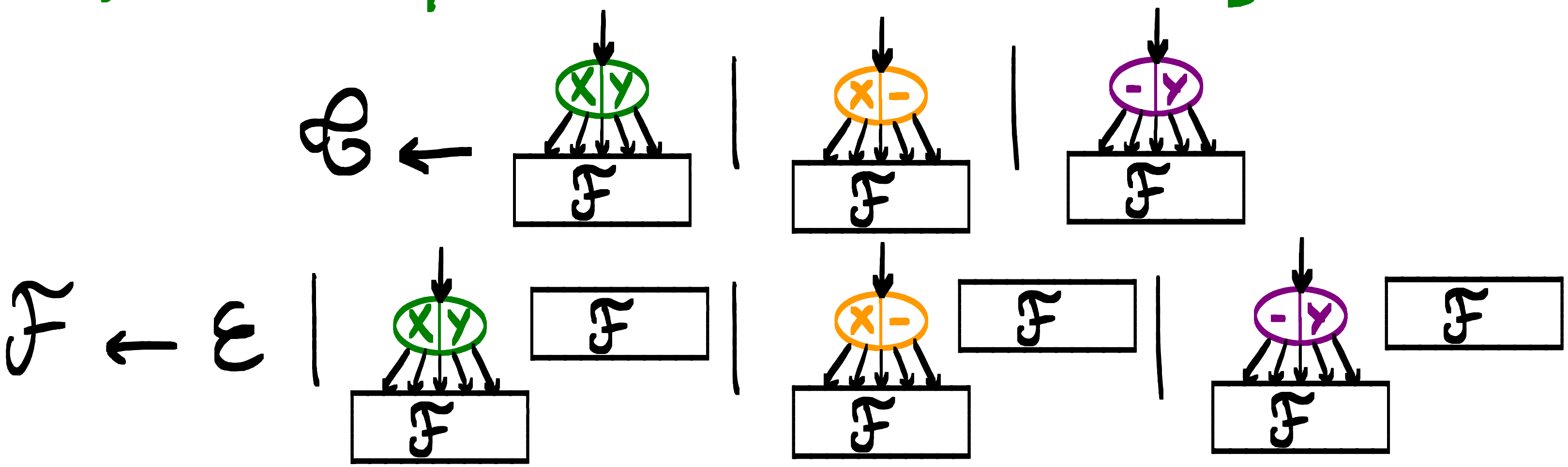
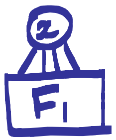
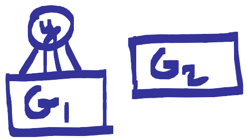
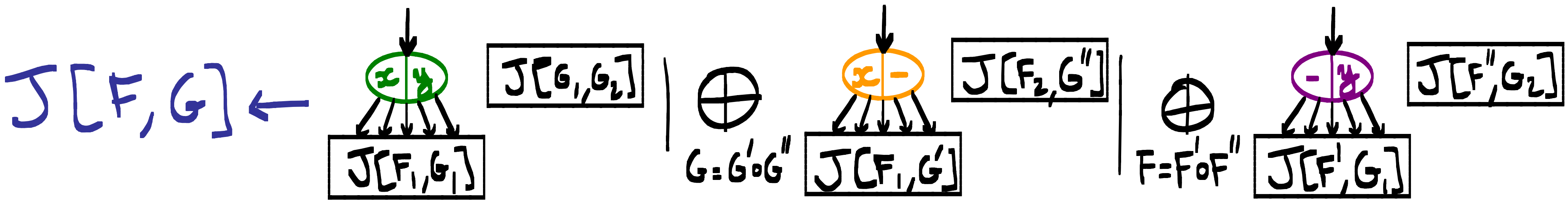


If F =  and G = , then



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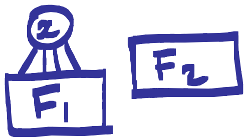
- If $F =$ 

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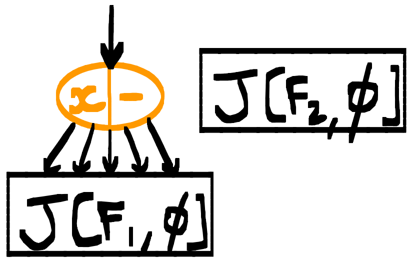
$J[F,G] \leftarrow$ 

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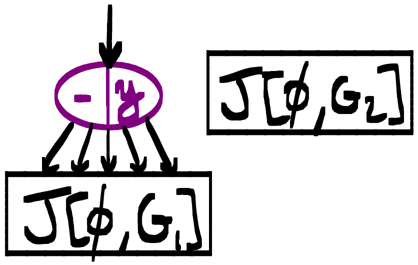
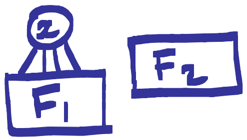
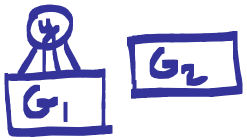
$J[F,G] \leftarrow$ 

- If $F =$ 

and $G =$ 

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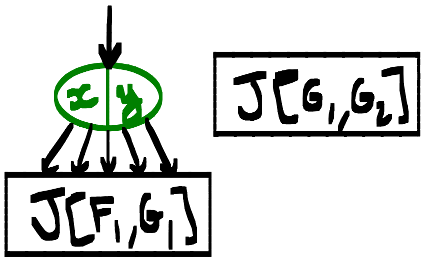
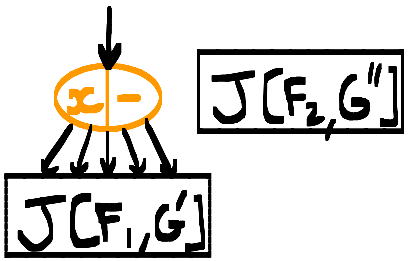
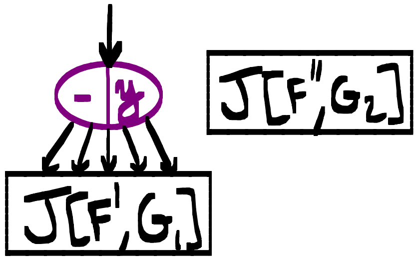
$J[F,G] \leftarrow$ 

$\mid \bigoplus_{G = G' \circ G''}$ 

$\mid \bigoplus_{F = F' \circ F''}$ 

SAMPLING

Theorem Let S and T be two trees of size n_1 and n_2.
Sampling alignments between S and T under the Gibbs-Boltzmann distribution can be done with worst-case time and space complexities $O(n_1 n_2 (n_1 + n_2)^2)$ and with average-case time and space complexities $O(n_1 n_2)$.

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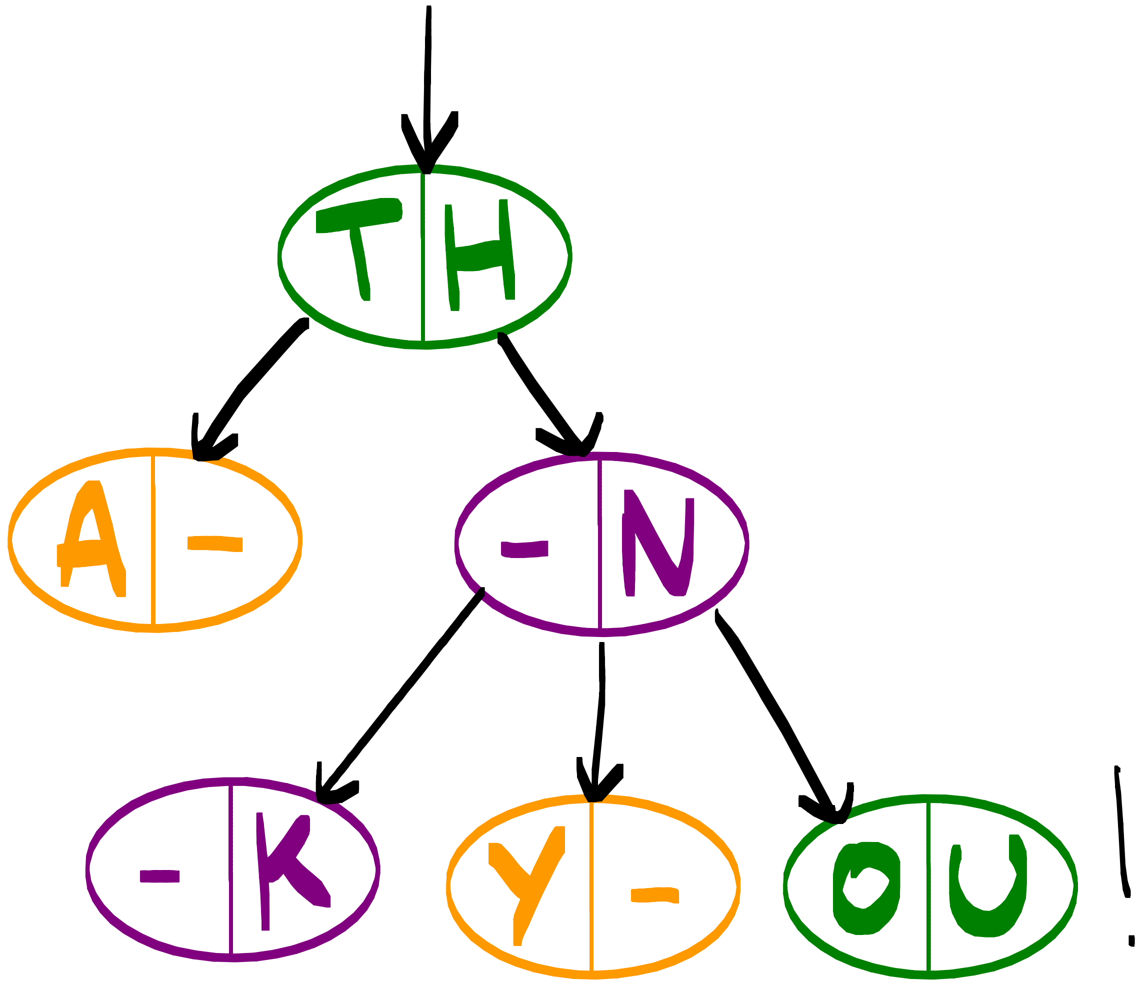
Proof inspired by

[Herrbach, Denise, Dulucq]

CONCLUSION

→ We are using our grammar and adapted dynamic programming algorithms to revisit the 3D alignments of RNA structures.

→ more general method?
new way to design dynamic programming algorithms?



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