Factor Graph Grammars for Probabilistic Modeling

Darcey Riley

2021-04-22

Mila Computational Calculus Reading Group

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Factor Graph Grammars (NeurIPS 2020)

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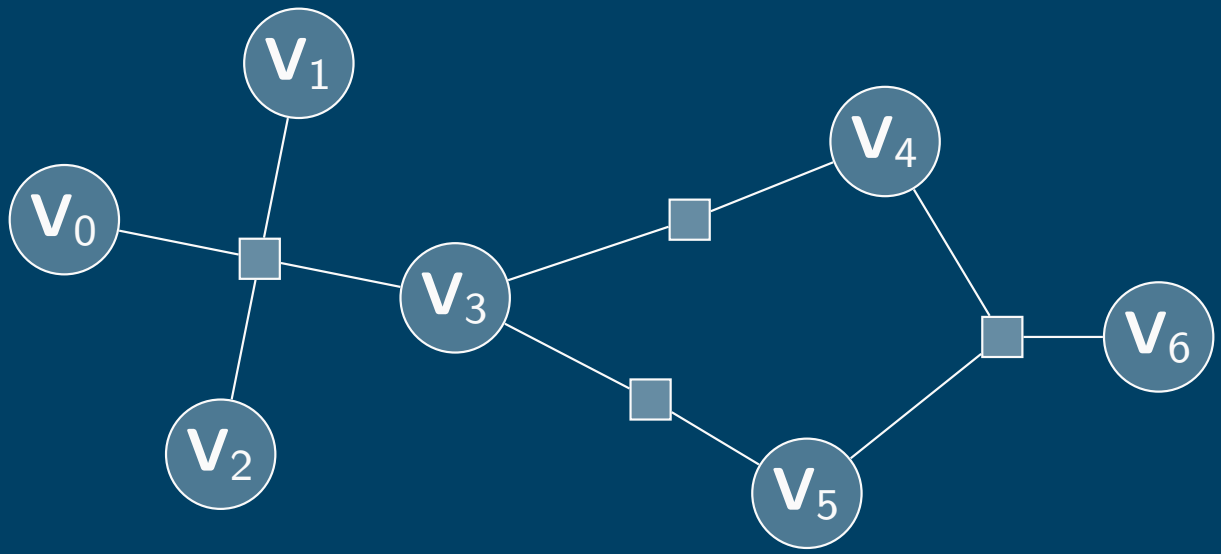
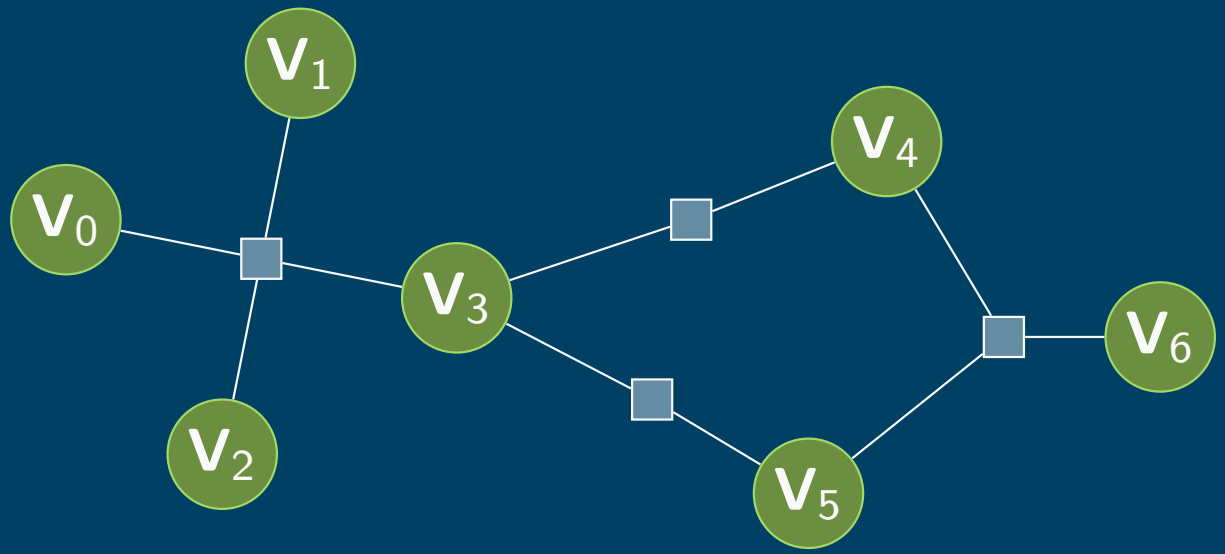
Chiang, David, and Darcey Riley. "Factor Graph Grammars." *Advances in Neural Information Processing Systems* 33 (2020).

Factor Graphs and Their Limitations

Factor Graphs

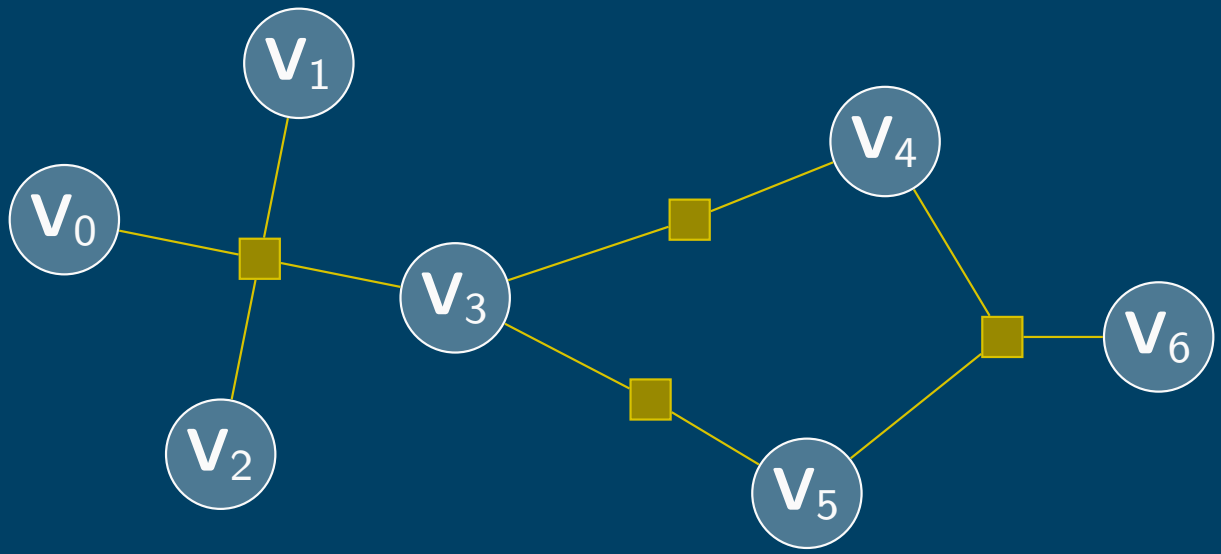


Factor Graphs



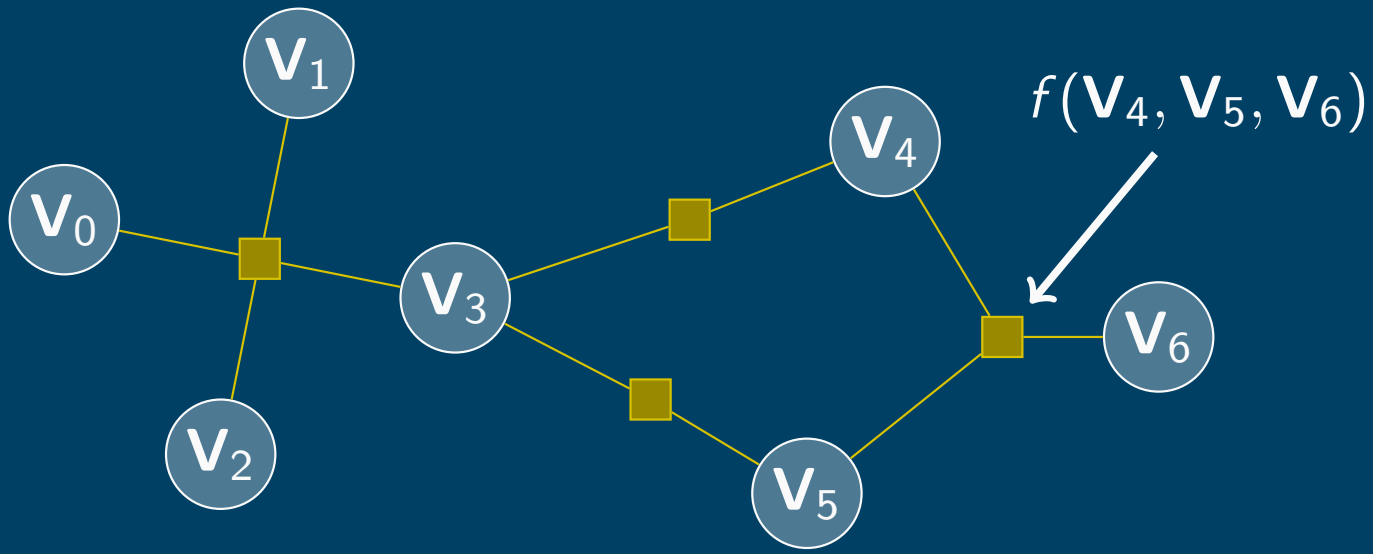
variables

Factor Graphs



factors

Factor Graphs



factors

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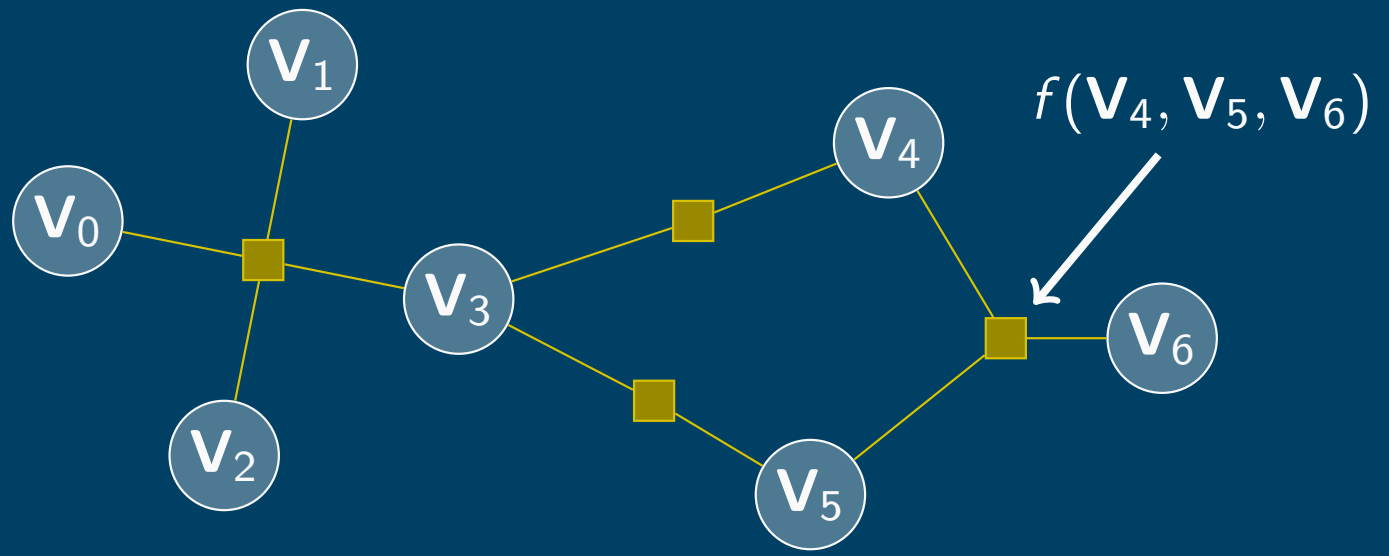
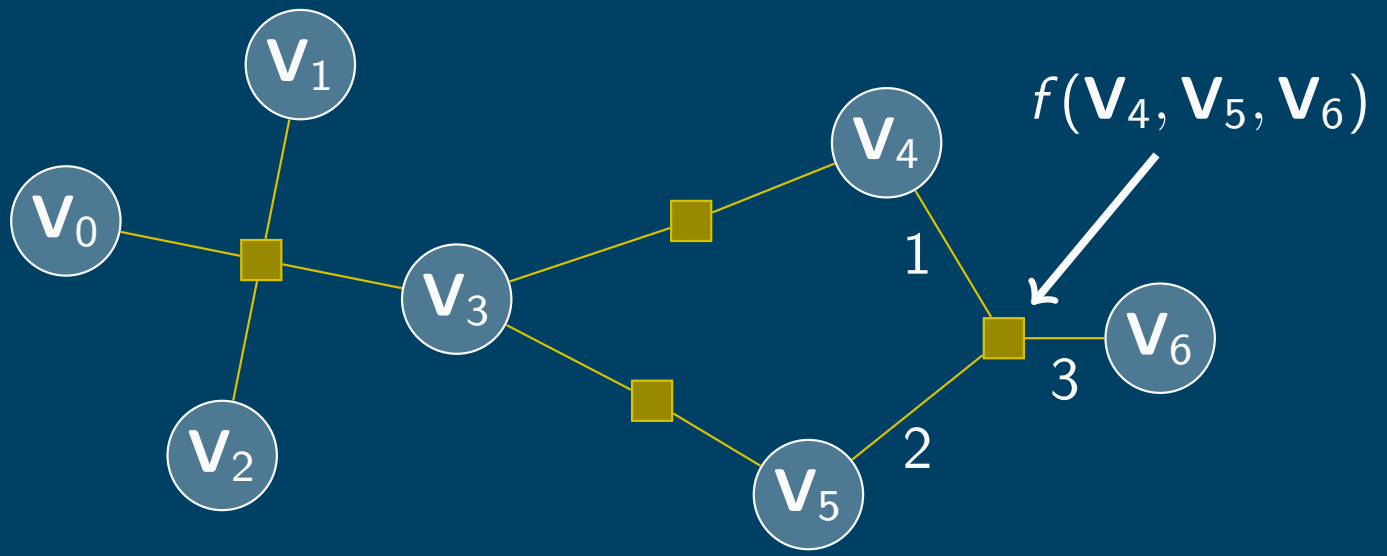


factors (hyperedges)

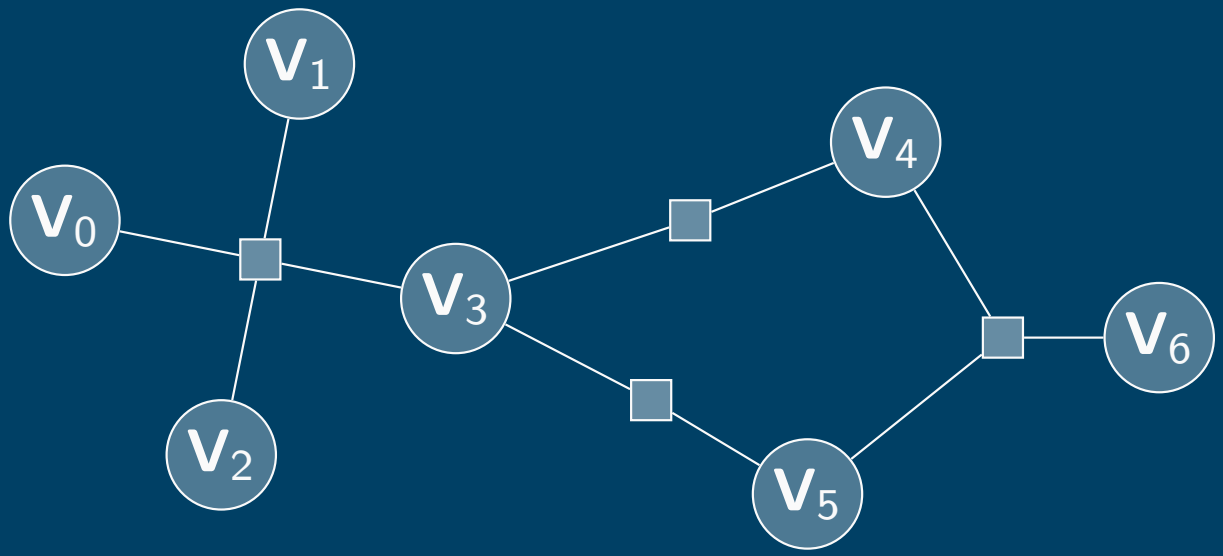
Factor Graphs



factors
(hyperedges)

Computing Probabilities

H:



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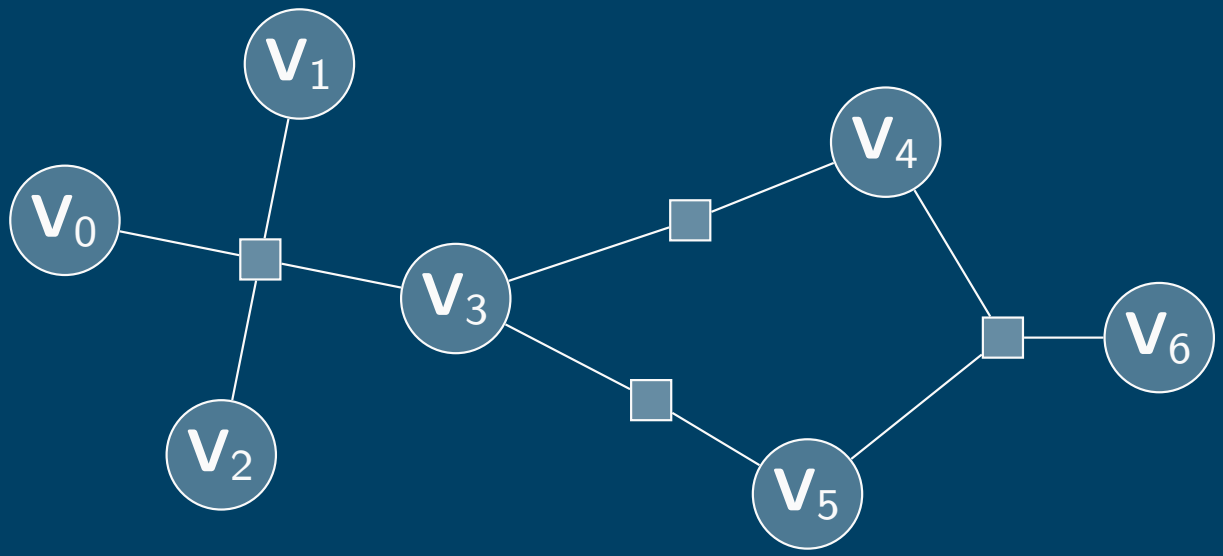
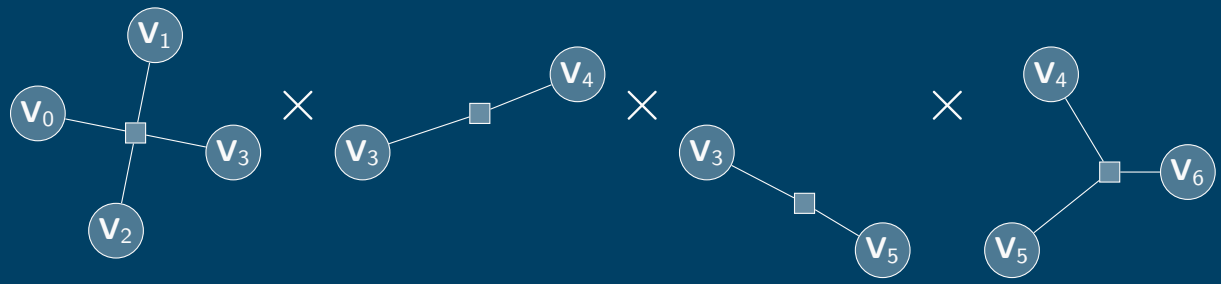
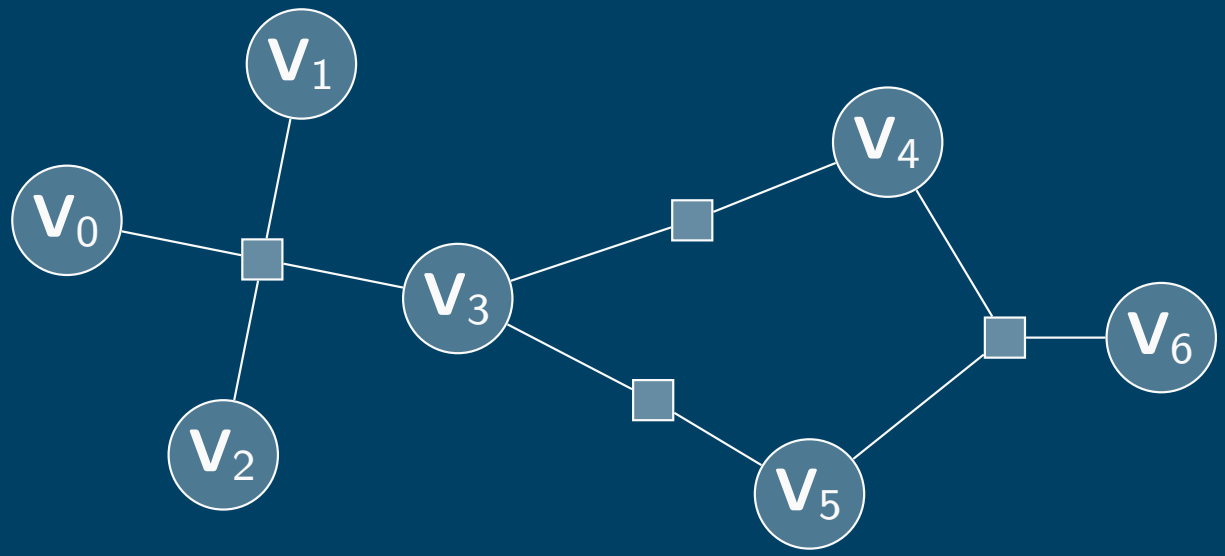




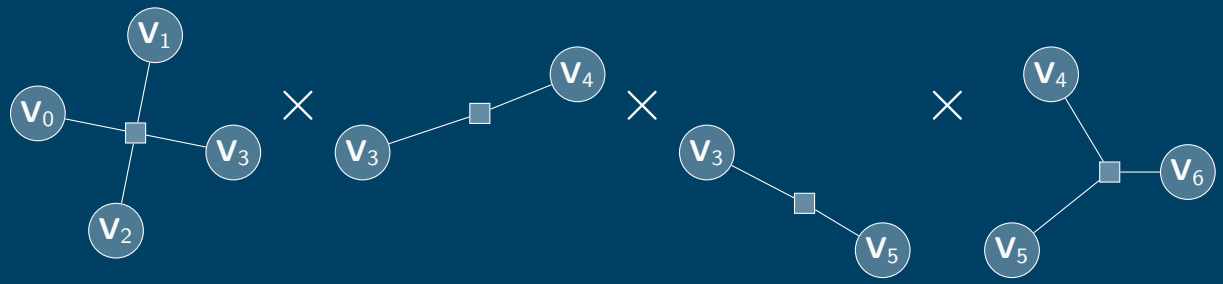
To compute weight of assignment: multiply factors together

Computing Probabilities

H:



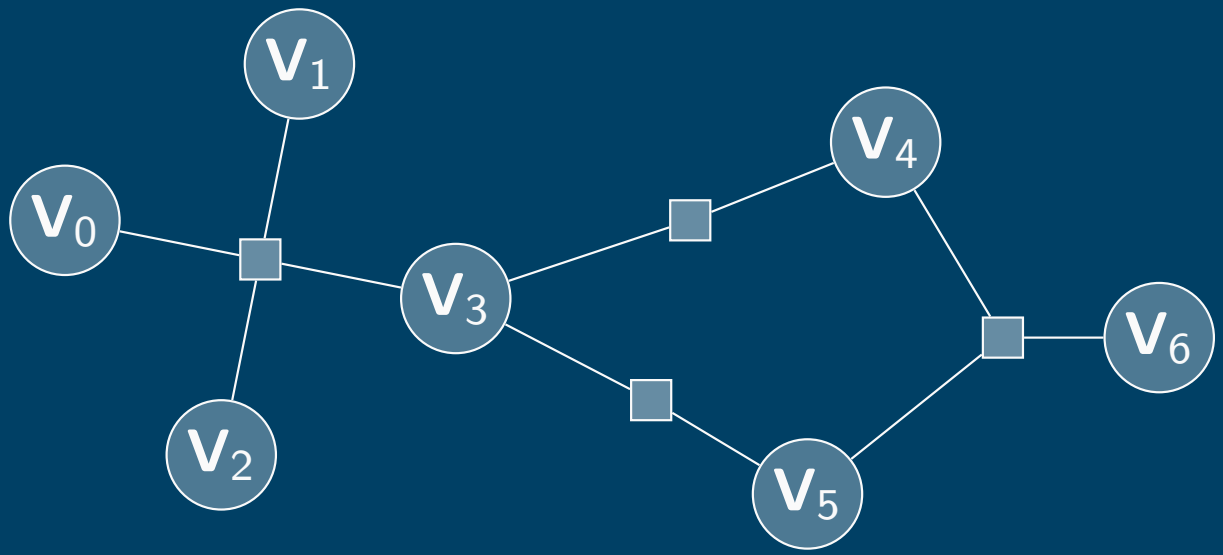
$$\frac{1}{Z}$$



To convert weight to probability: divide by normalizing constant Z

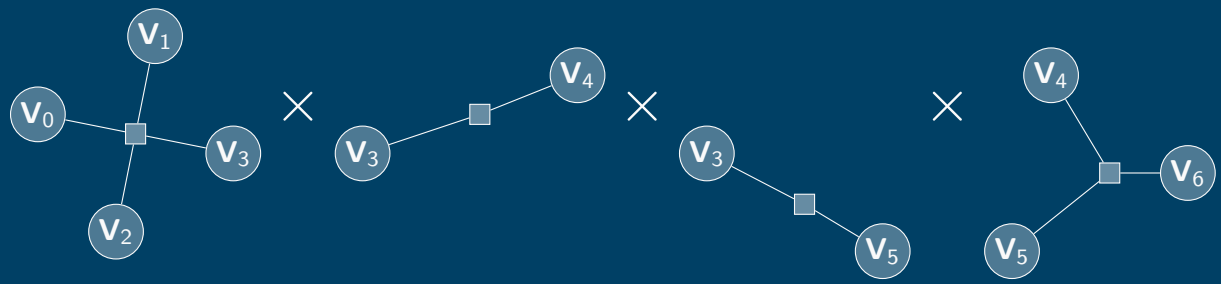
Computing Probabilities

H:



$Z(H) =$

$$\sum_{\text{assignments to } V_0, V_1, \ldots, V_6}$$

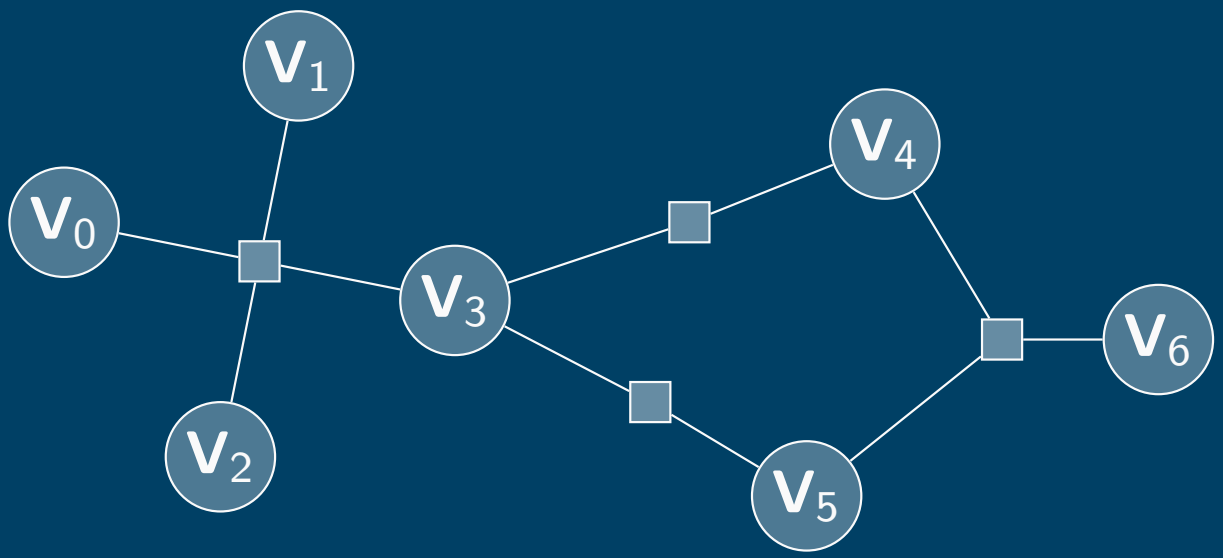


To compute normalizing constant: sum over the weights of all assignments

Limitations

Factor graphs are powerful...

...but they are limited by their fixed structure.



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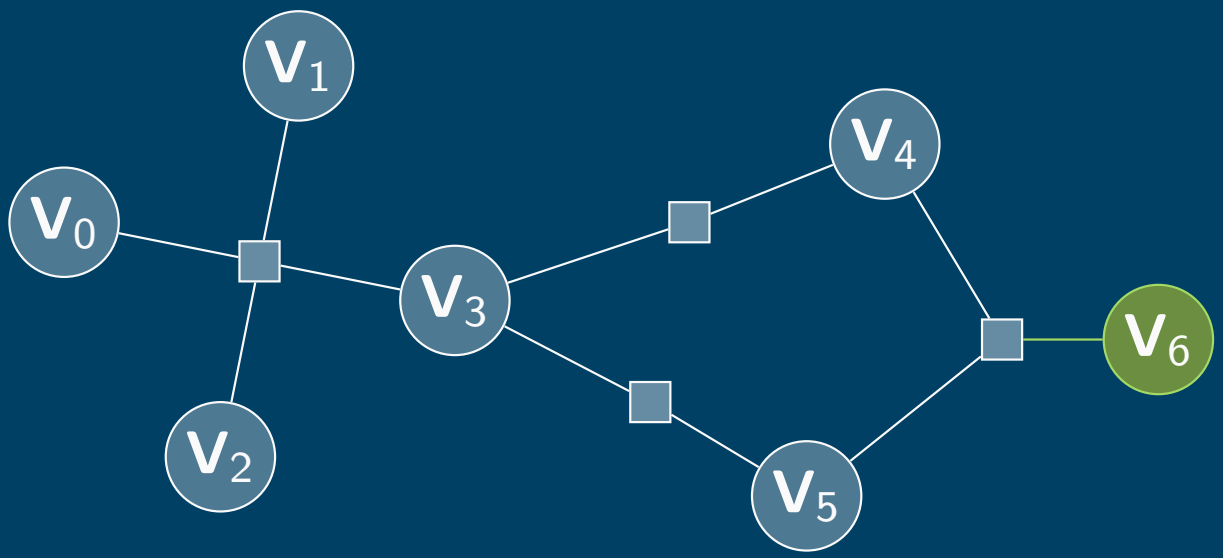

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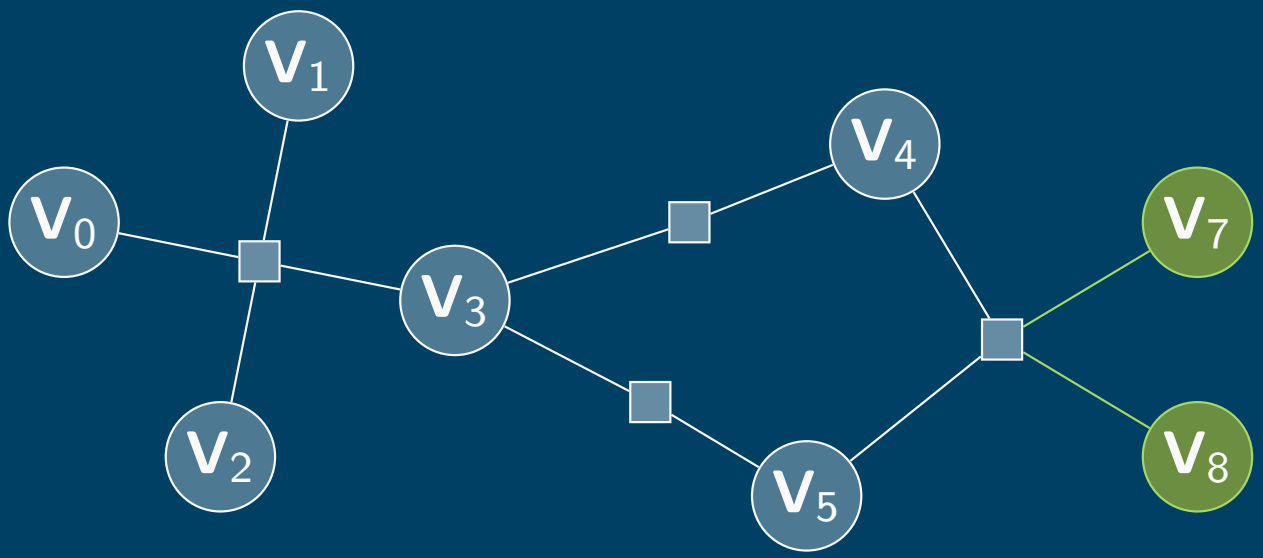

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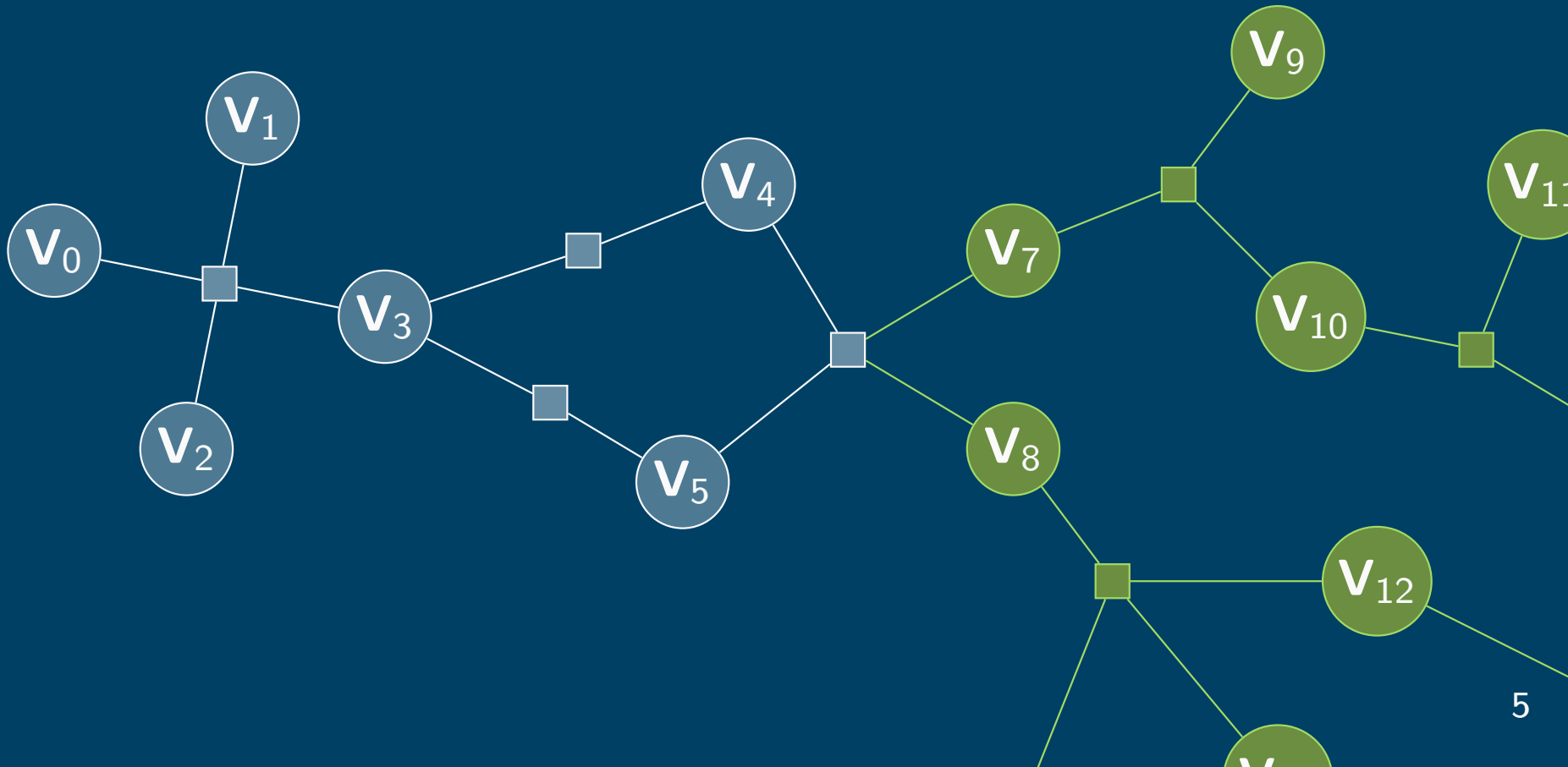

Limitations

Can't represent many models from NLP.

Want a probability model over all possible sentences:

The dog was eating spaghetti.

I hate getting a flat tire.

Nobody wears orange pajamas while playing the accordion.

⋮

These sentences have unbounded length.

Limitations

Can't represent HMMs:

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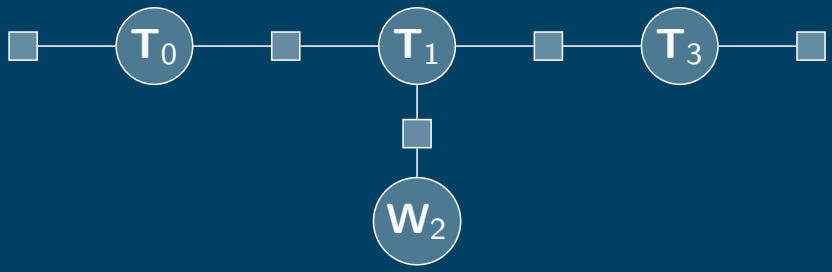

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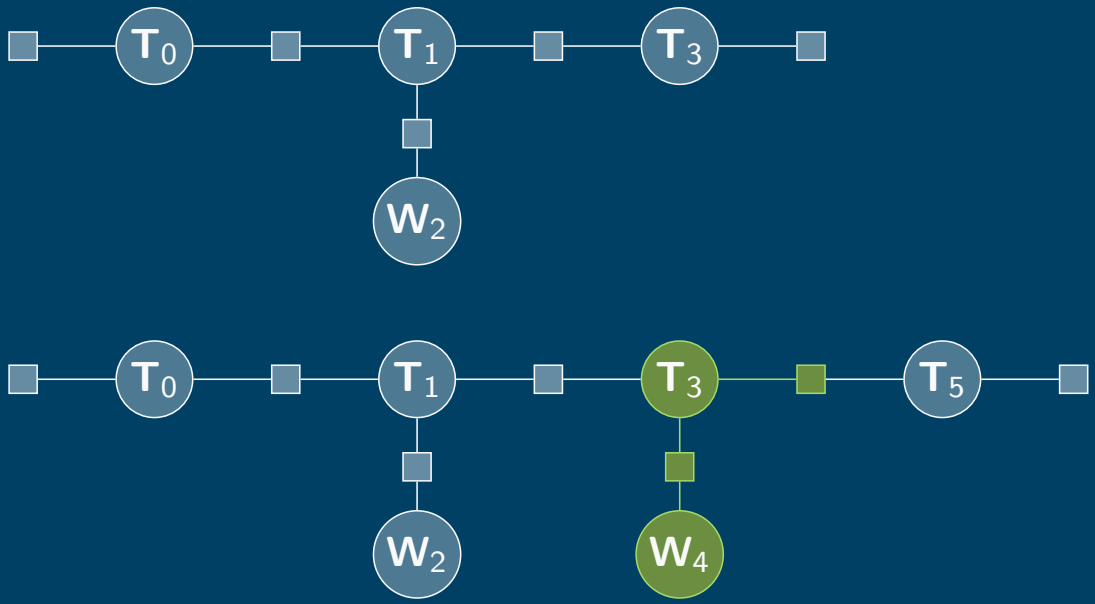

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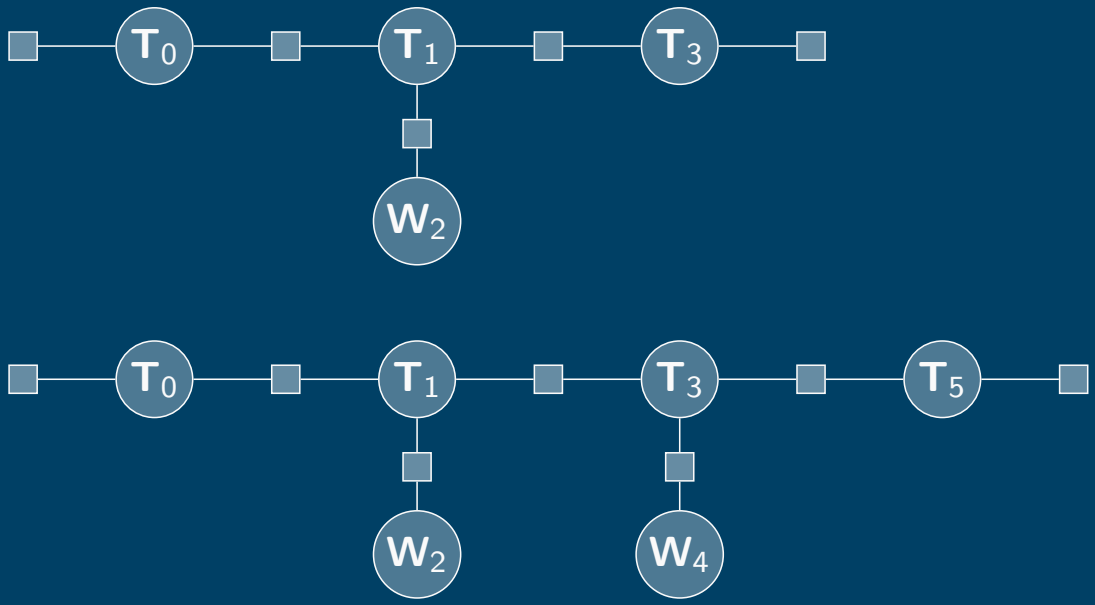

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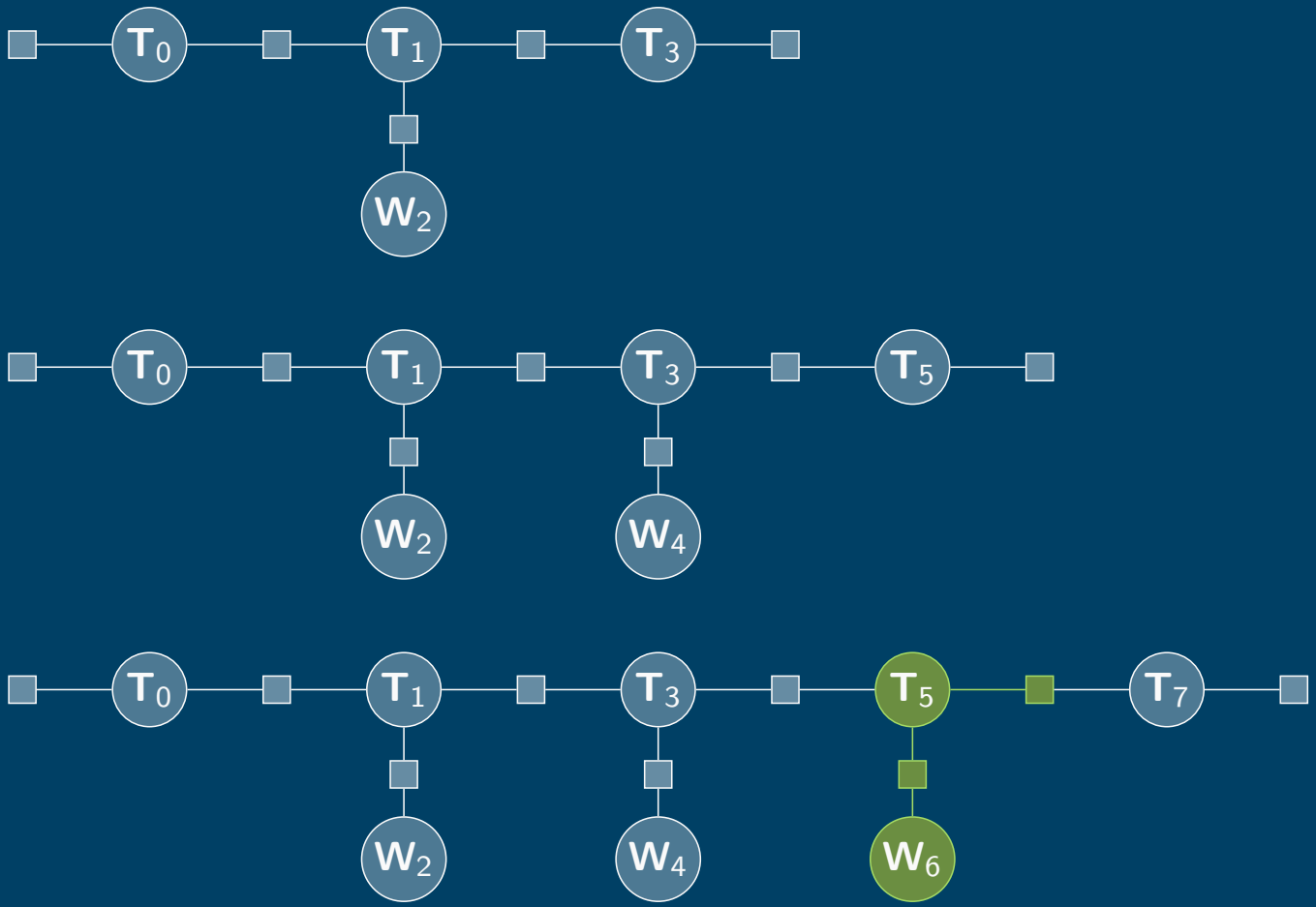

Limitations

Can't represent PCFGs:

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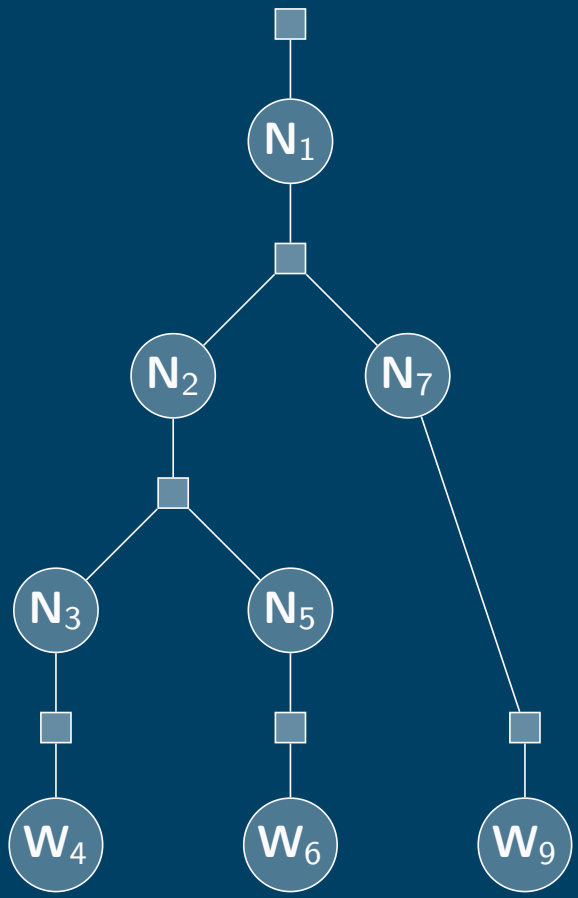
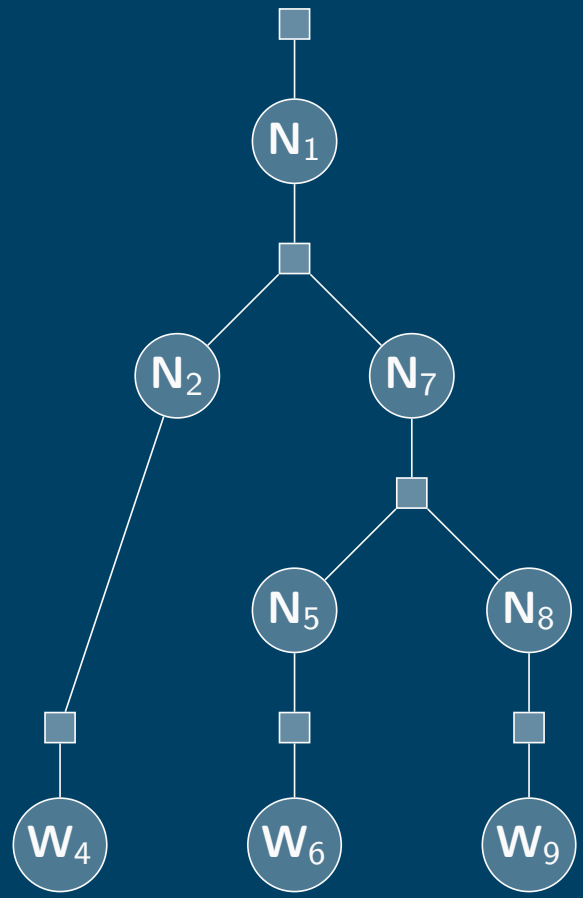




Solution

Use hyperedge replacement grammars

(Bauderon and Courcelle, 1987; Habel and Kreowski, 1987)

to generate sets of factor graphs

Hyperedge Replacement Grammars

Review: Context-Free (String) Grammars

$$S \to TC$$
$$T \to aTb$$
$$T \to \epsilon$$
$$C \to cC$$
$$C \to \epsilon$$

generates the language
$\{a^n b^n c^m | n, m \geq 0\}$

S

TC

aTbC

aaTbbC

aaaTbbbC

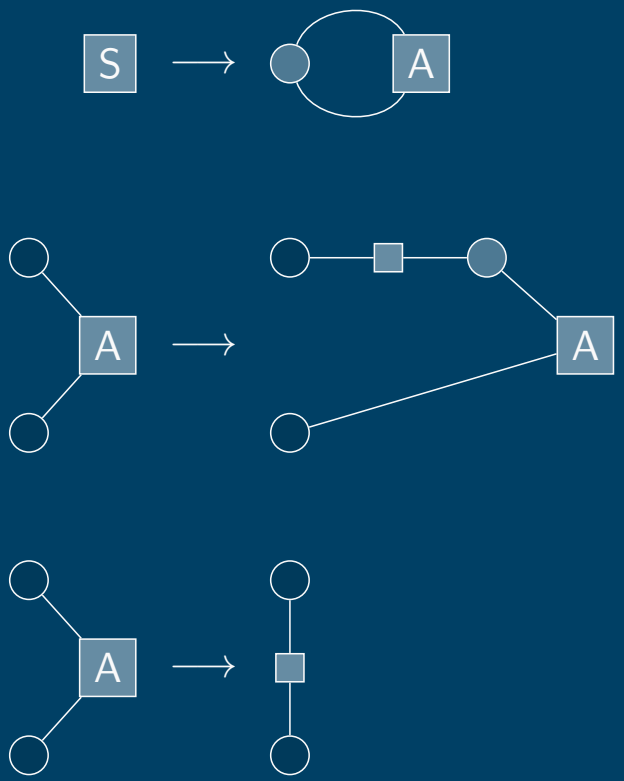
aaabbbC

aaabbbcC

aaabbbccC

aaabbbcc

Hyperedge Replacement Grammars: Example



generates the language
of ring graphs

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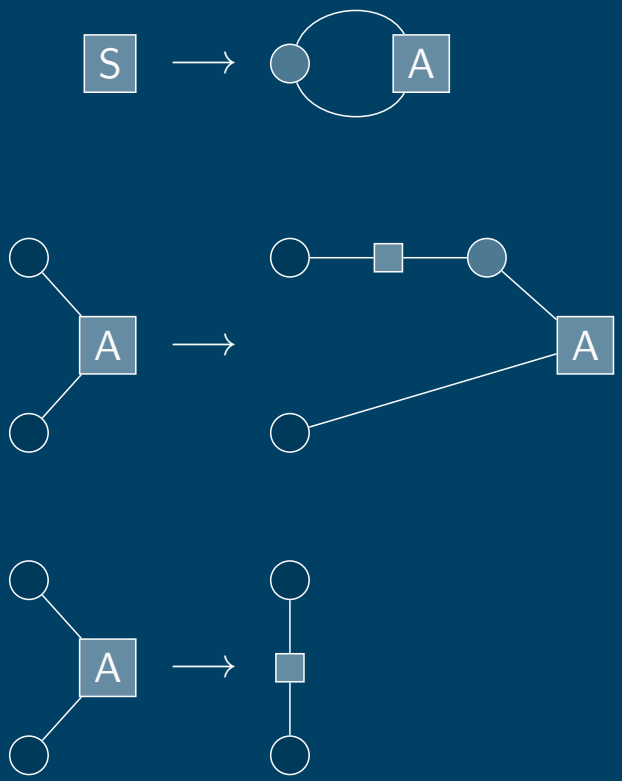

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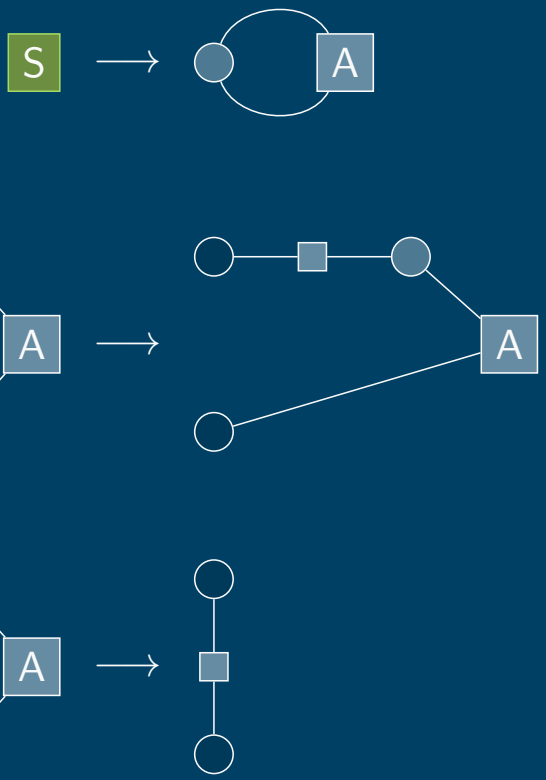

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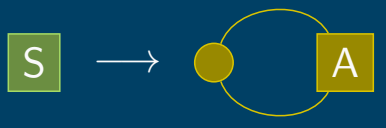

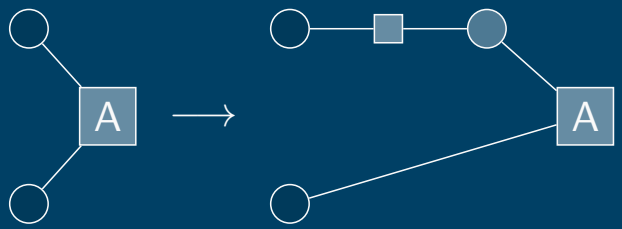

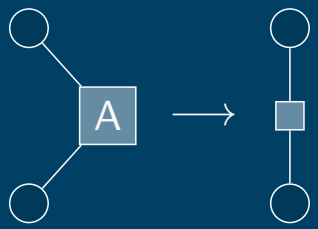

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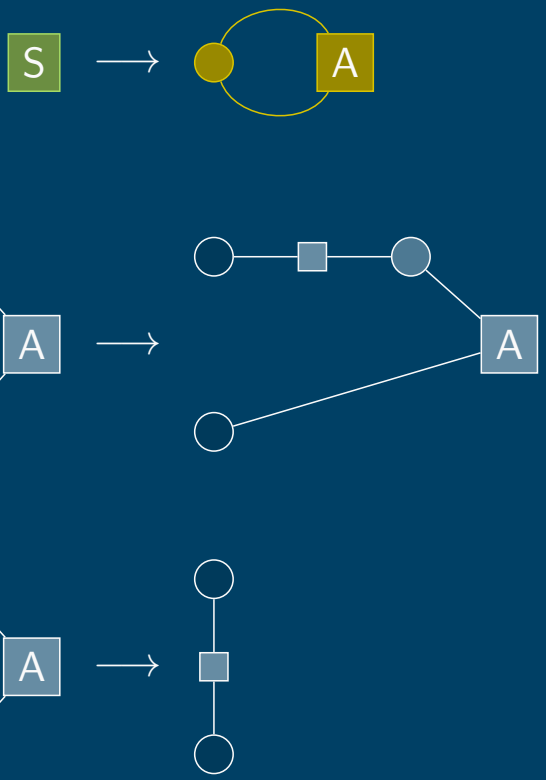

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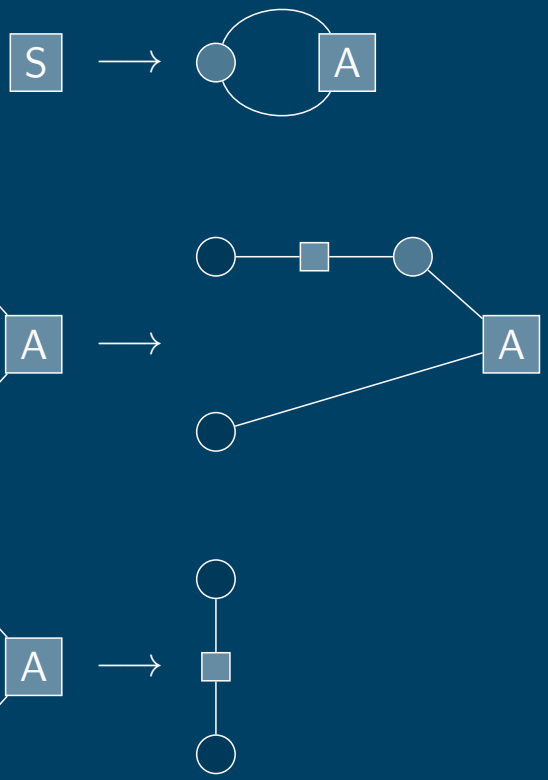

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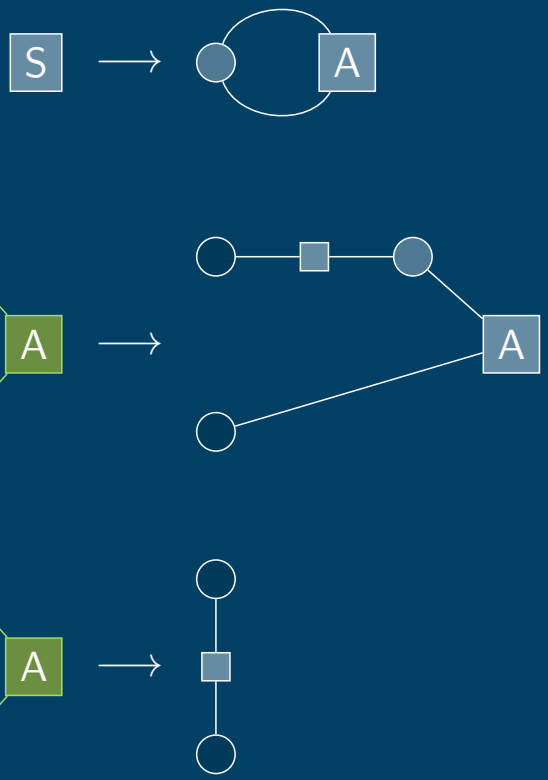

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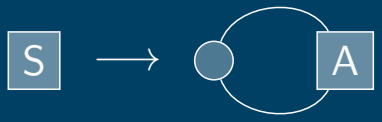

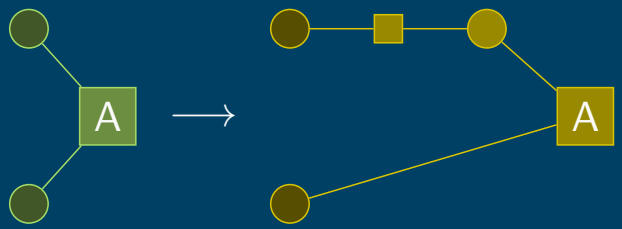

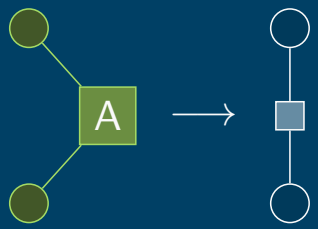

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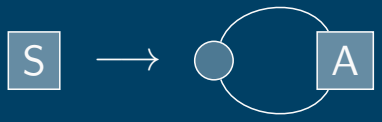

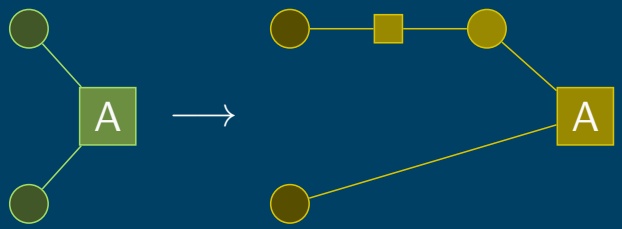

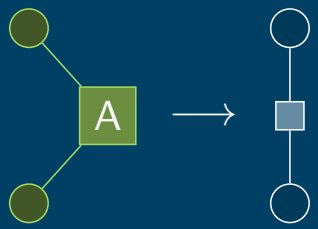

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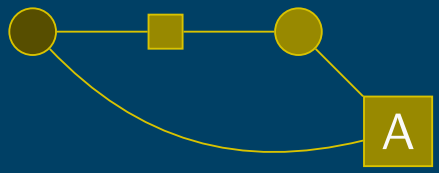

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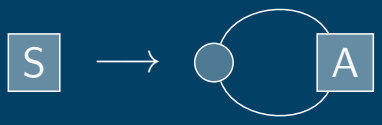

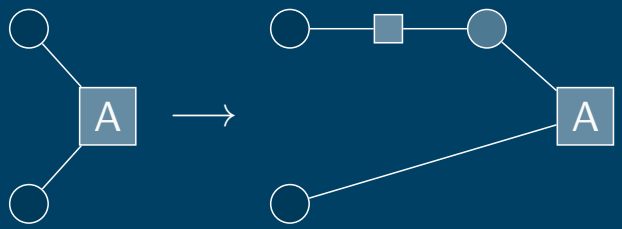

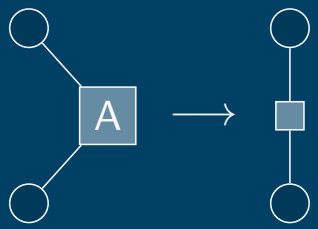

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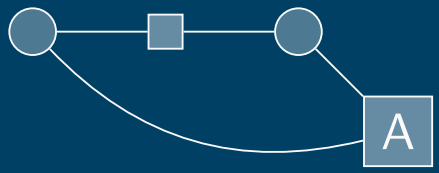

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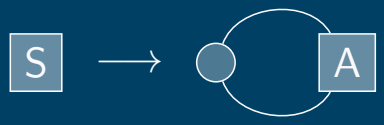

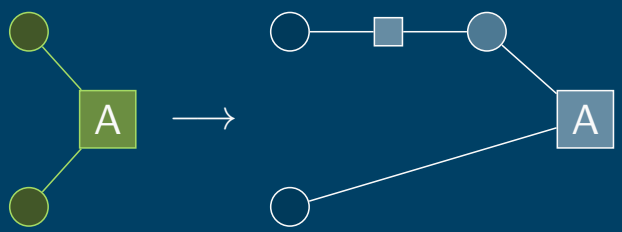

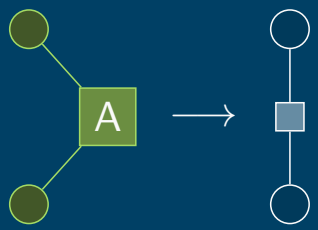

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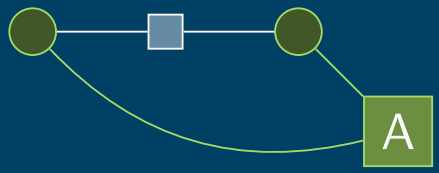

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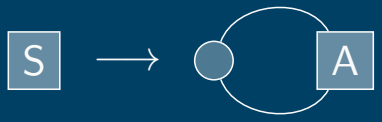

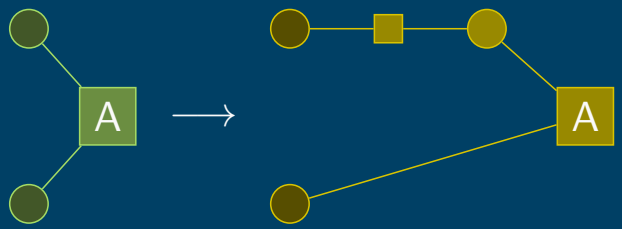

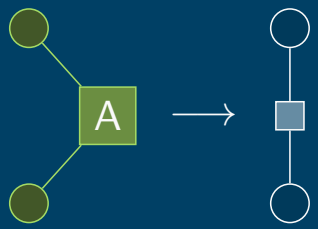

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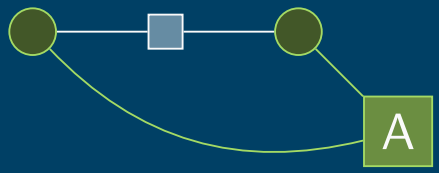

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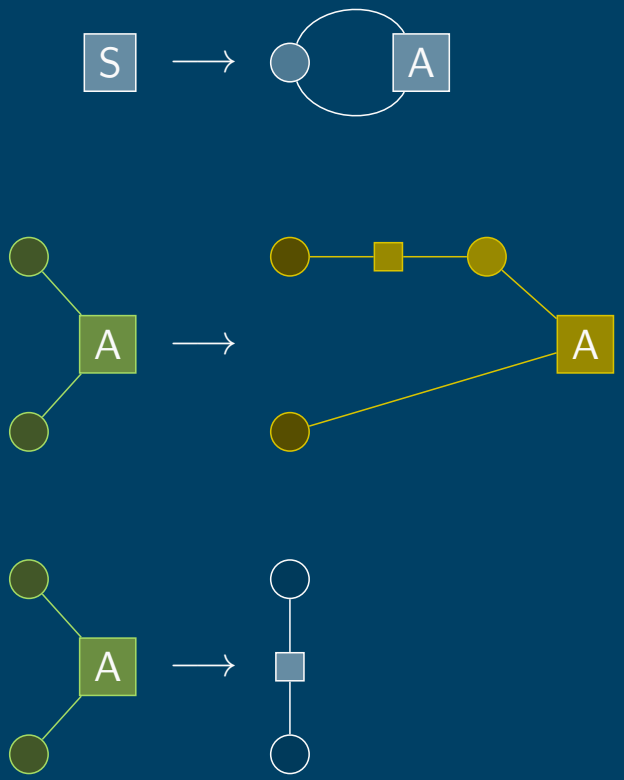

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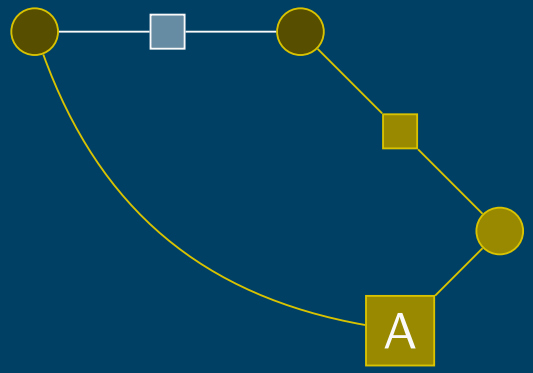

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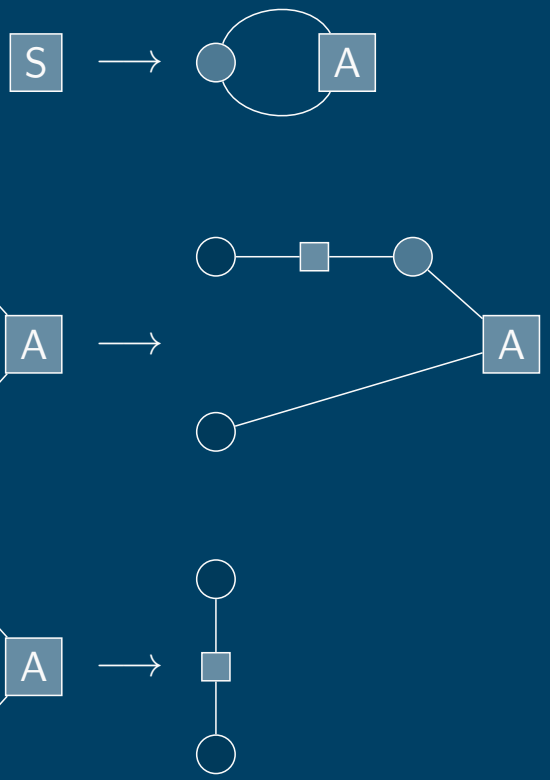

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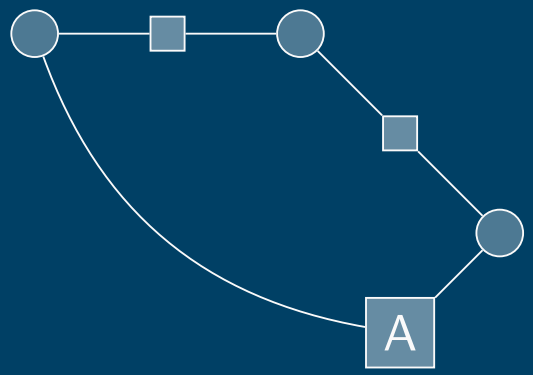
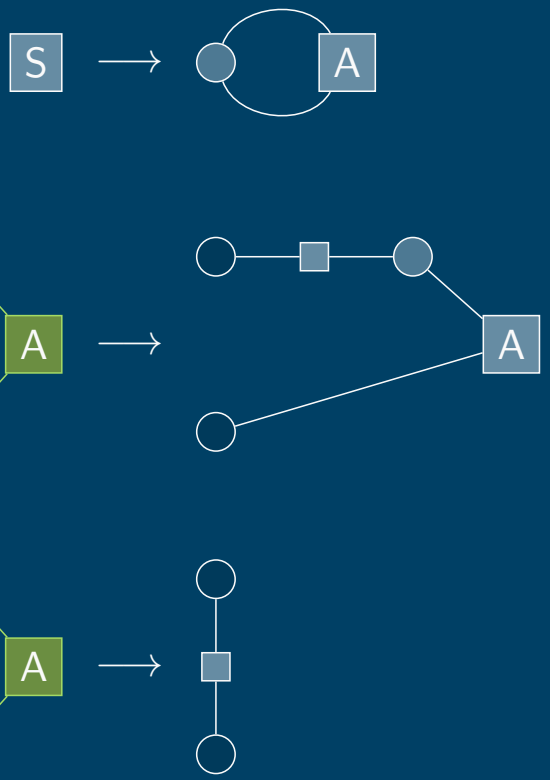


Hyperedge Replacement Grammars: Example



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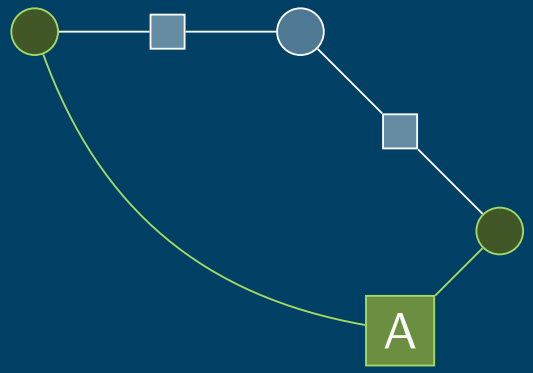

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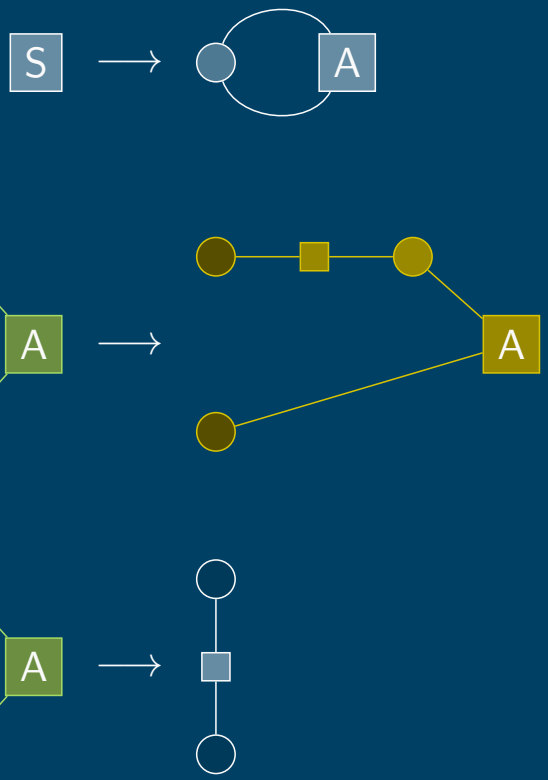

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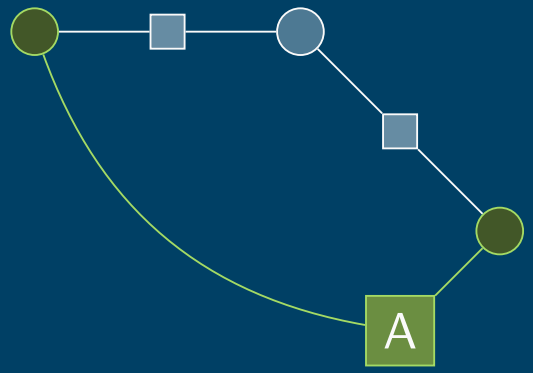

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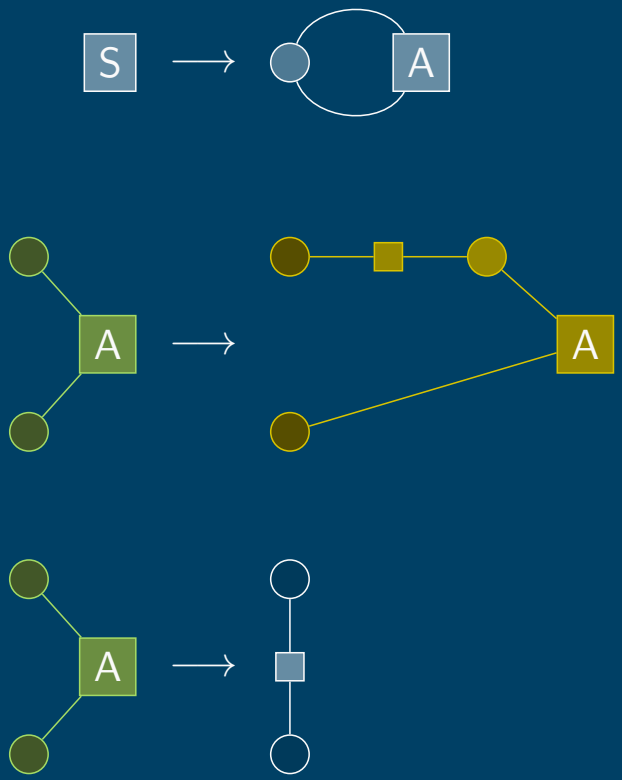

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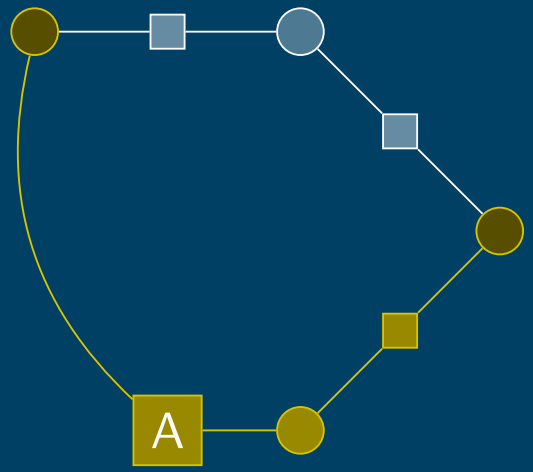

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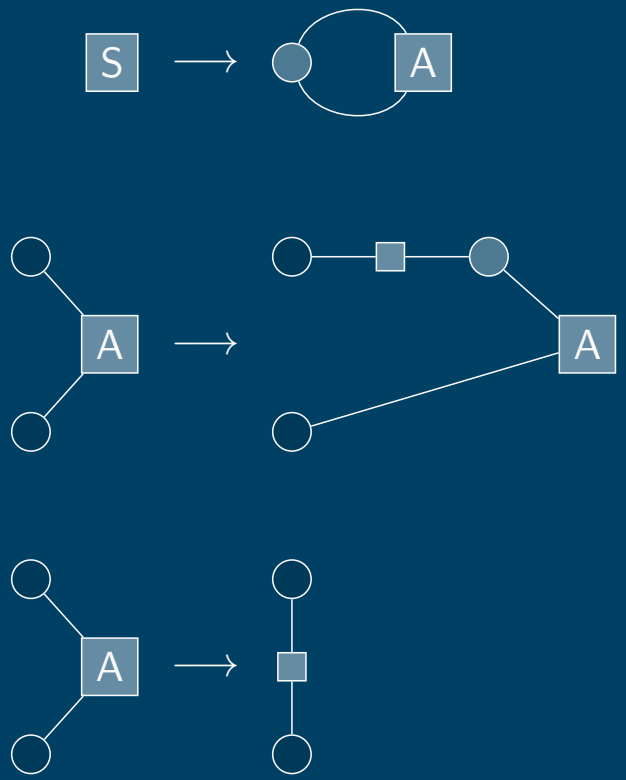

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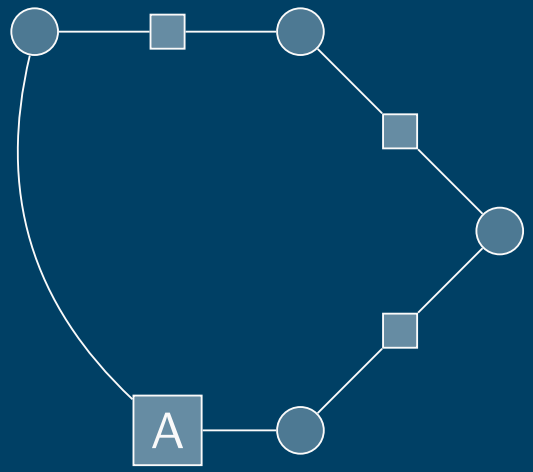

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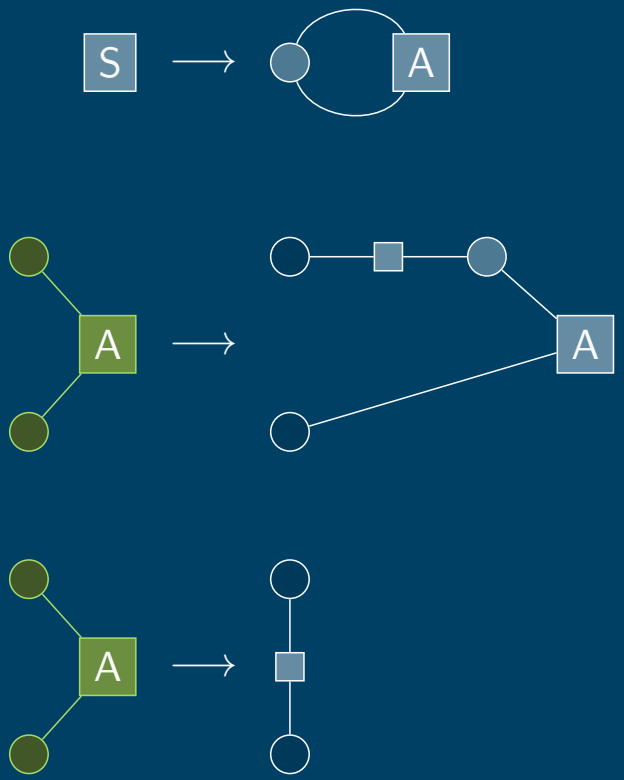

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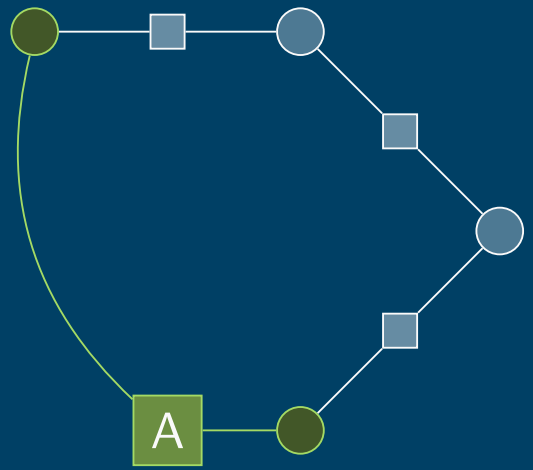

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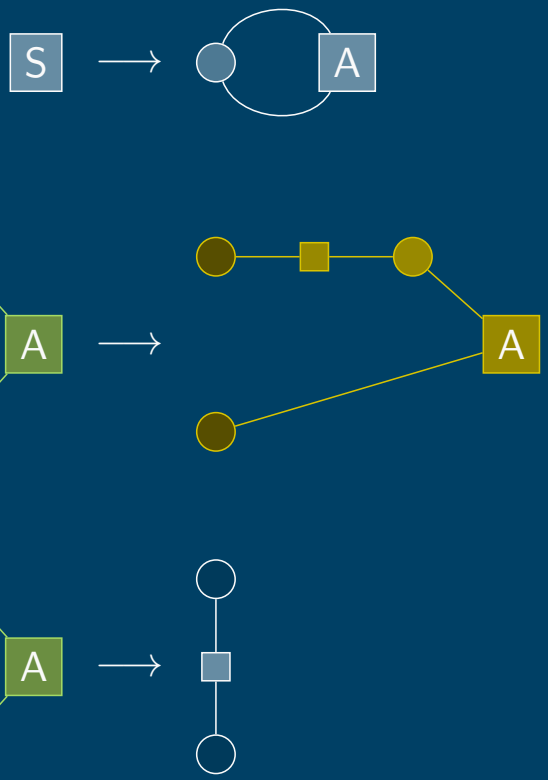

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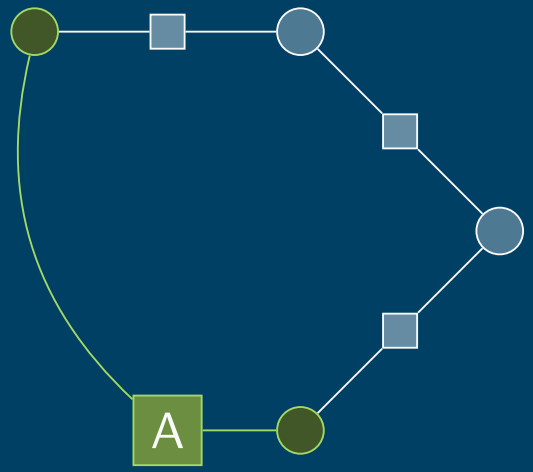

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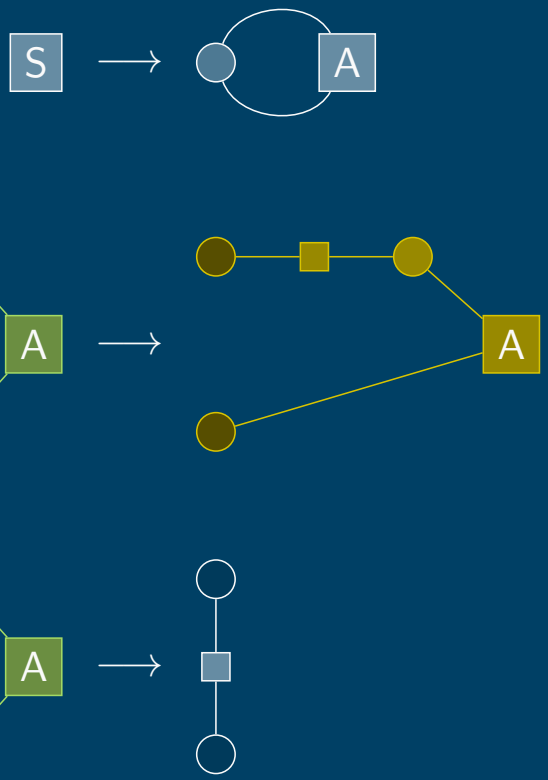

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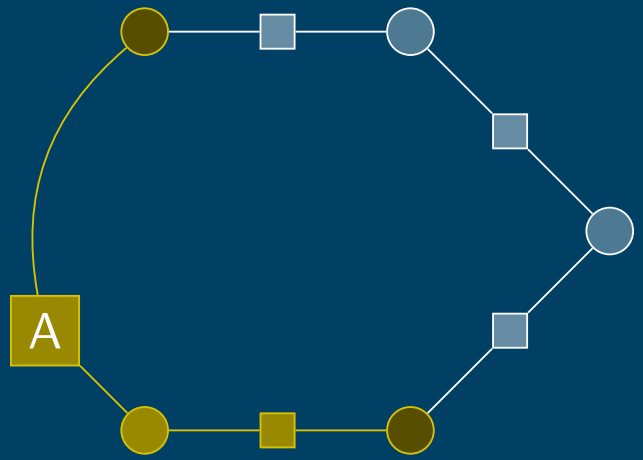

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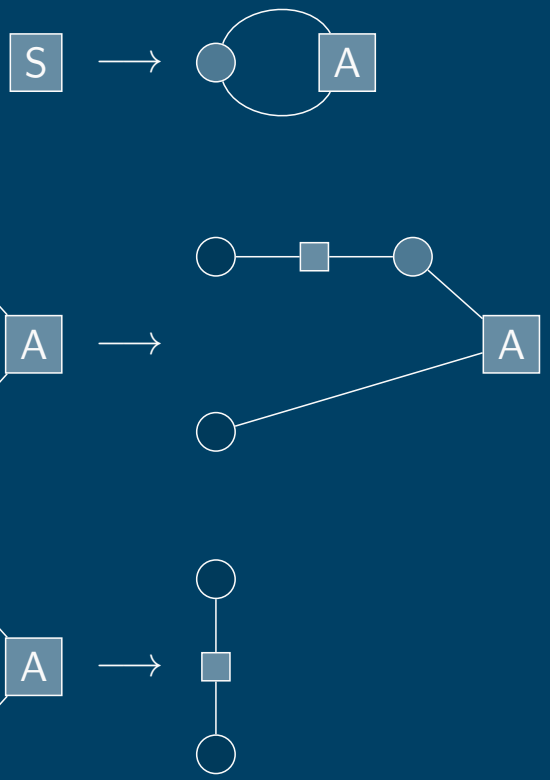

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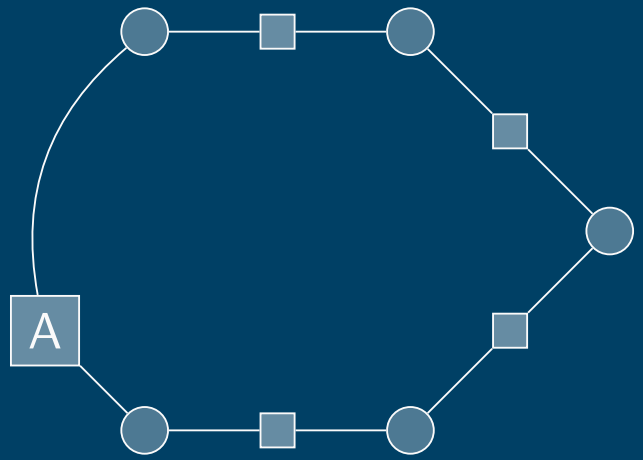

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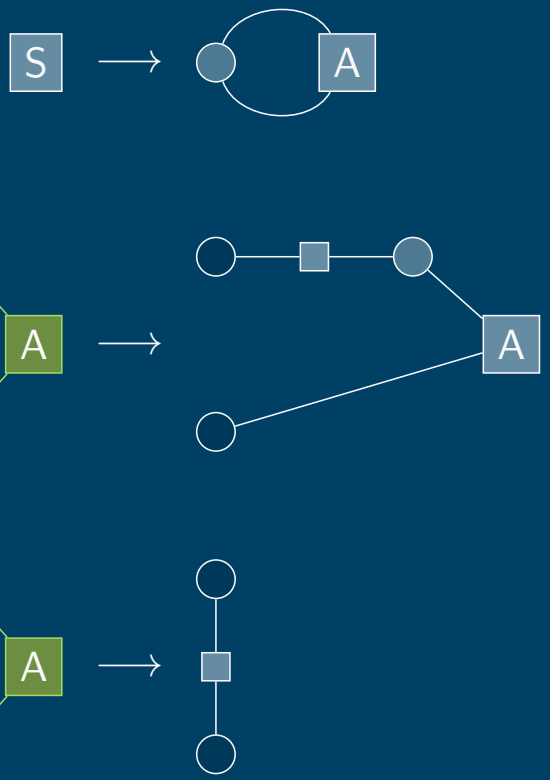

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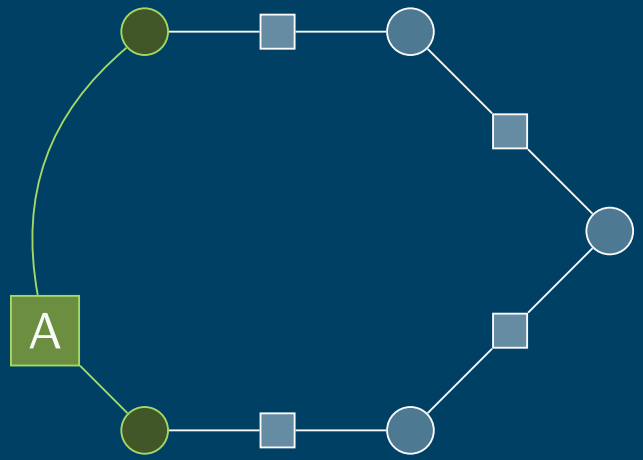

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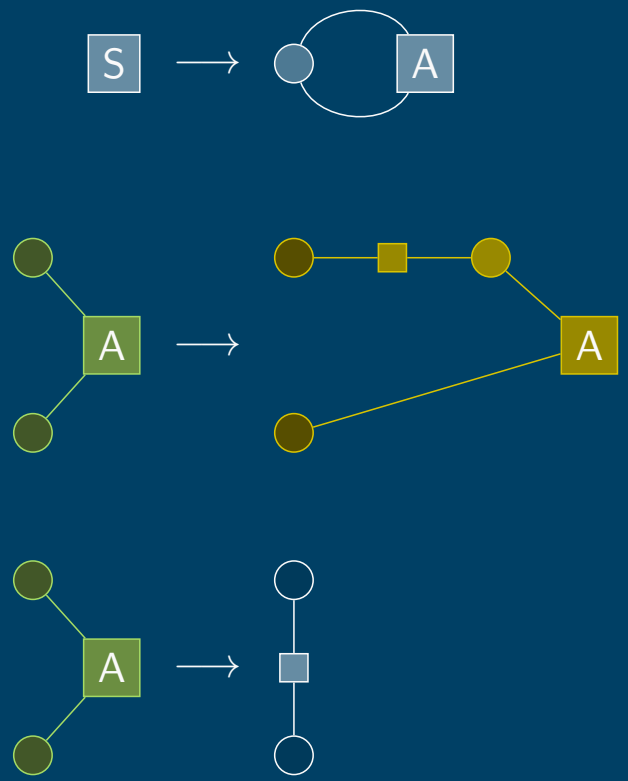

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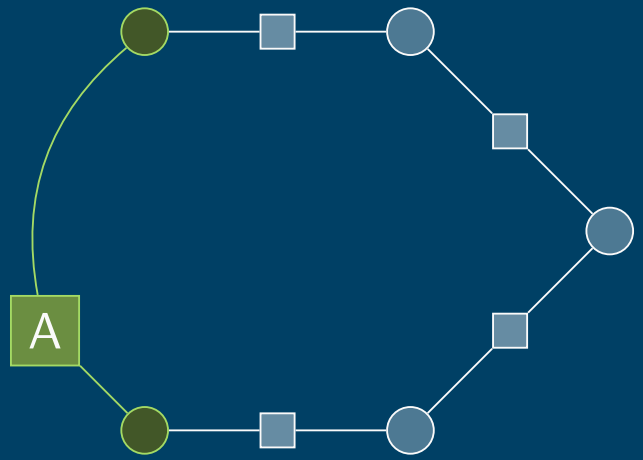

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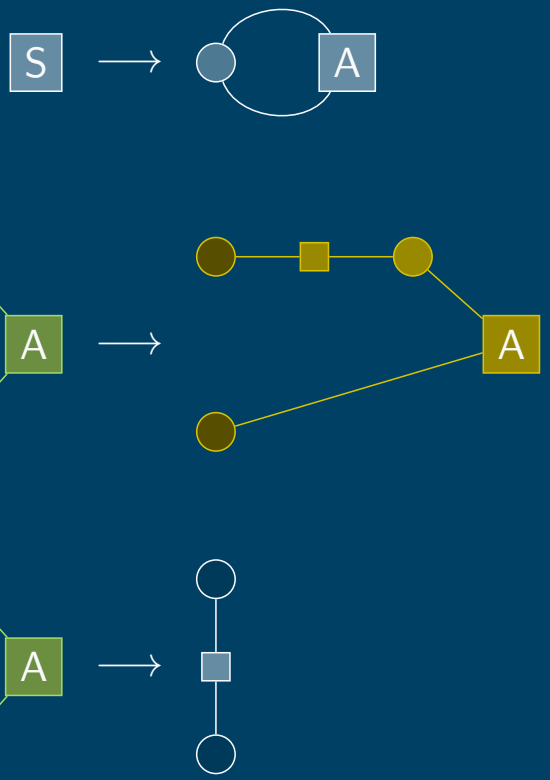

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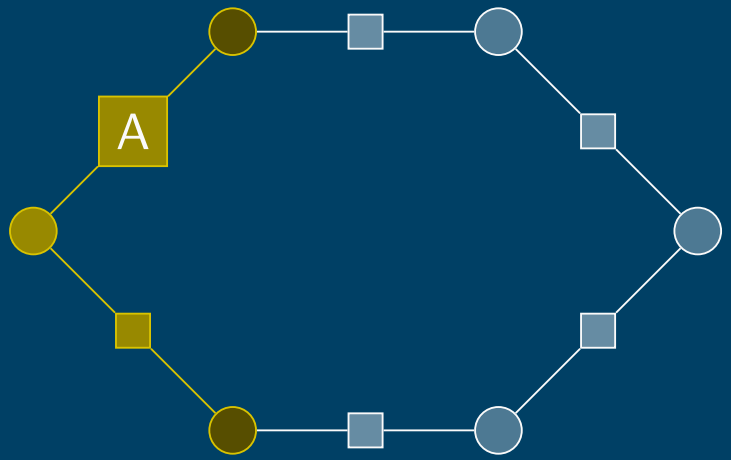

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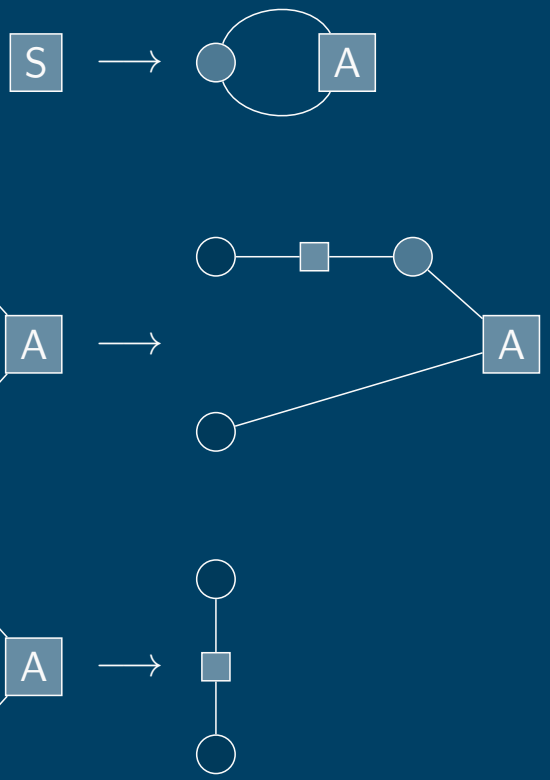

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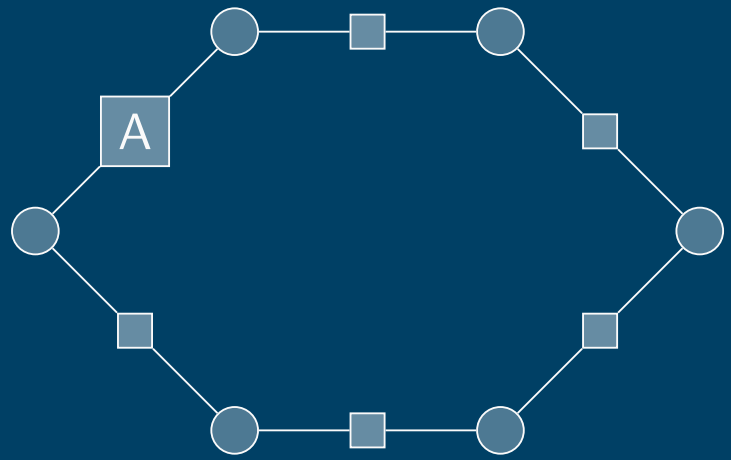

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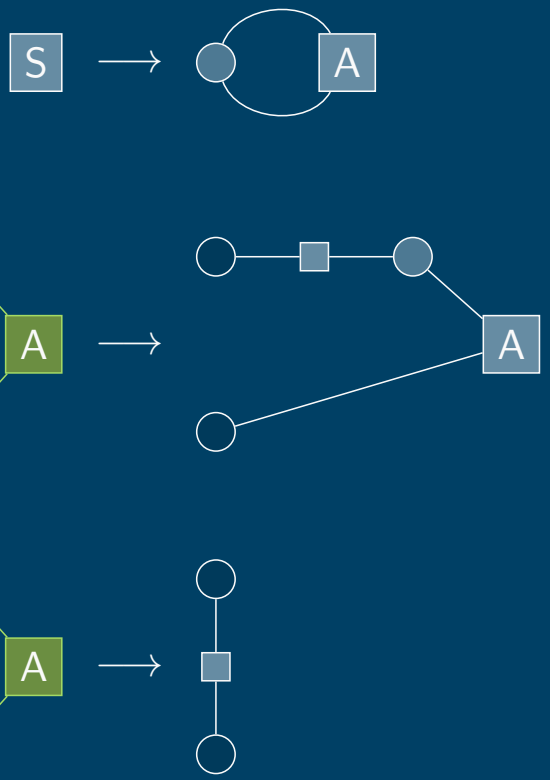

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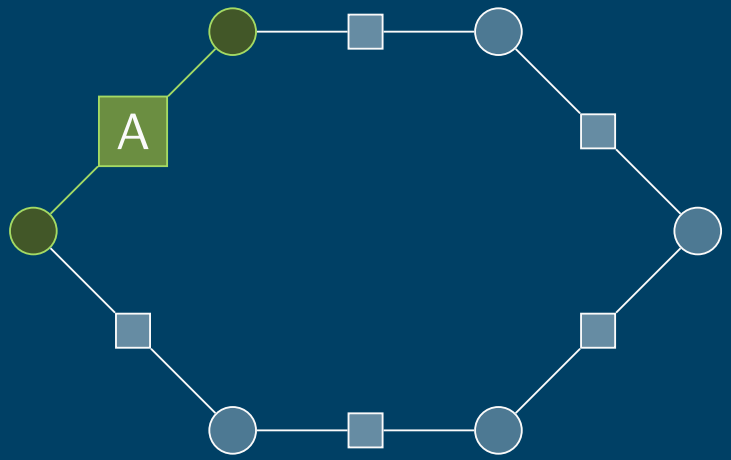

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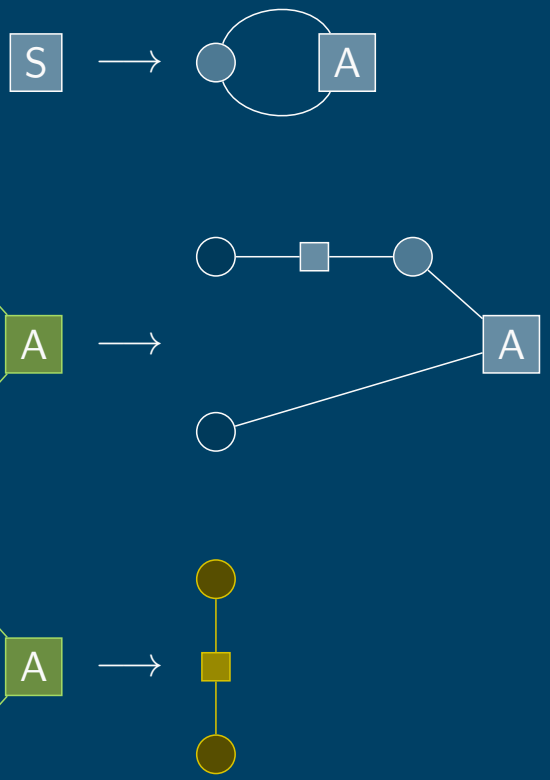

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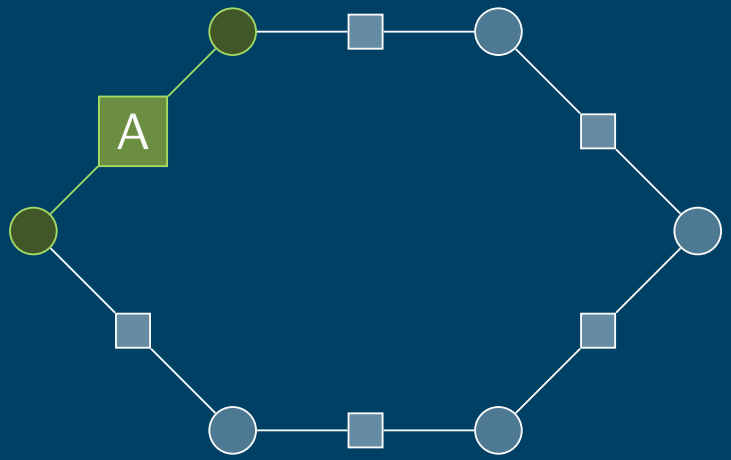

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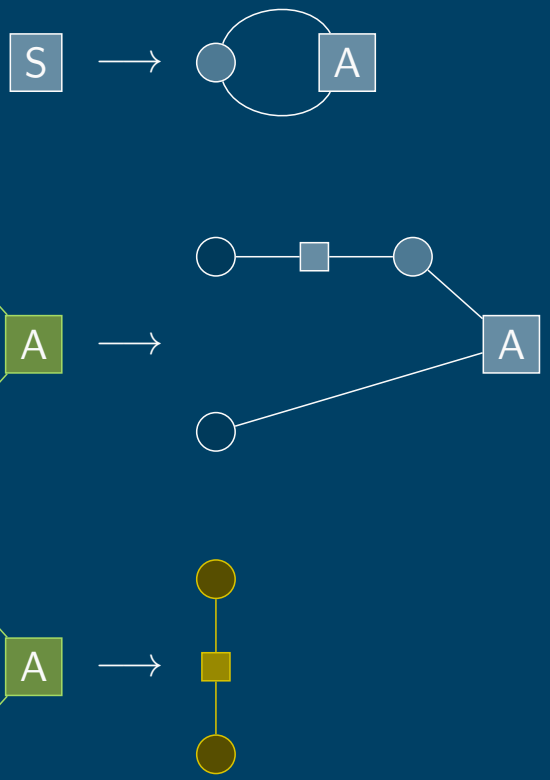

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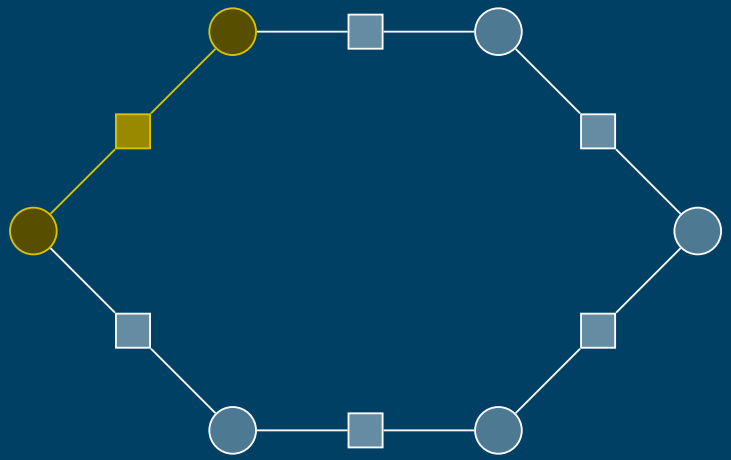

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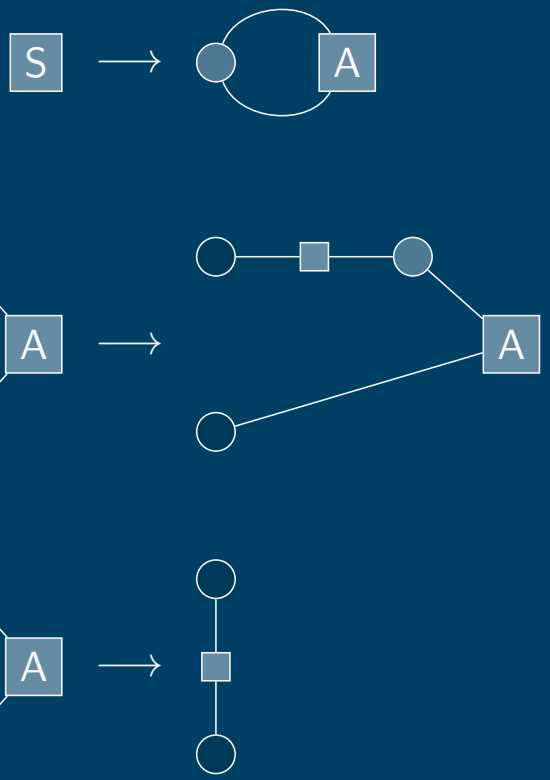

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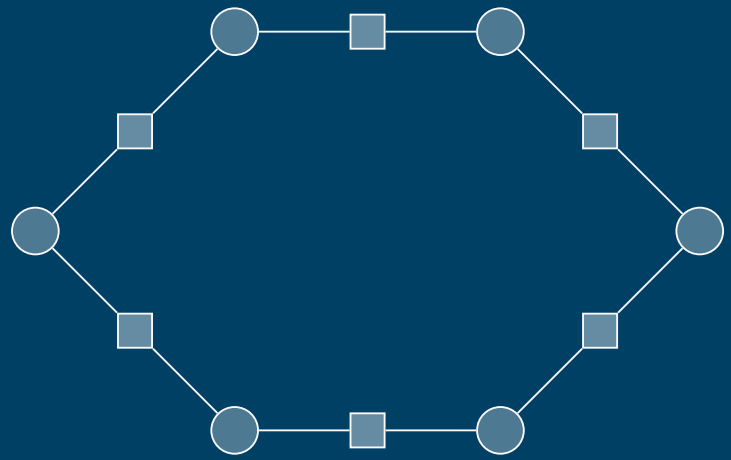

Factor Graph Grammars

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A factor graph grammar

is a hyperedge replacement grammar

that generates factor graphs

A Factor Graph Grammar for HMMs

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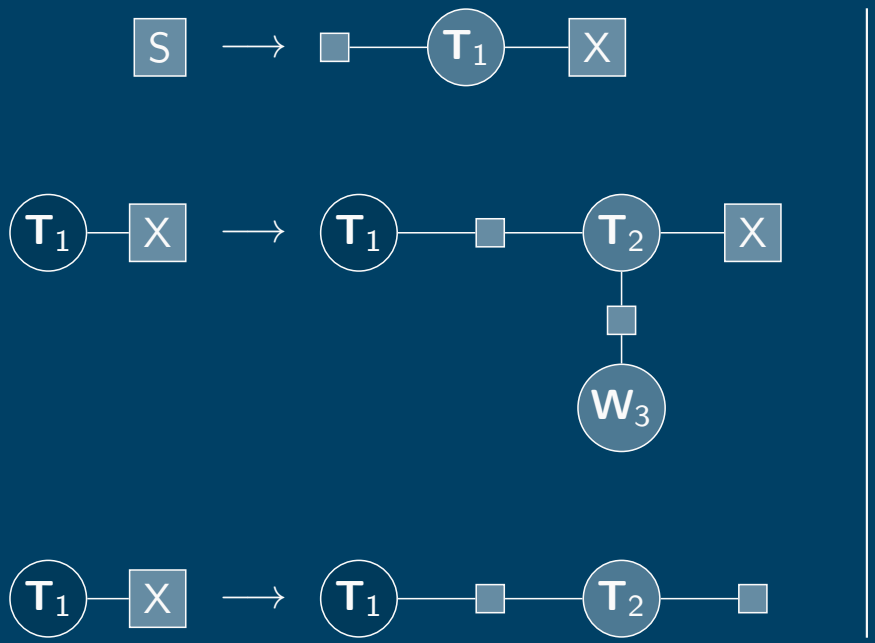

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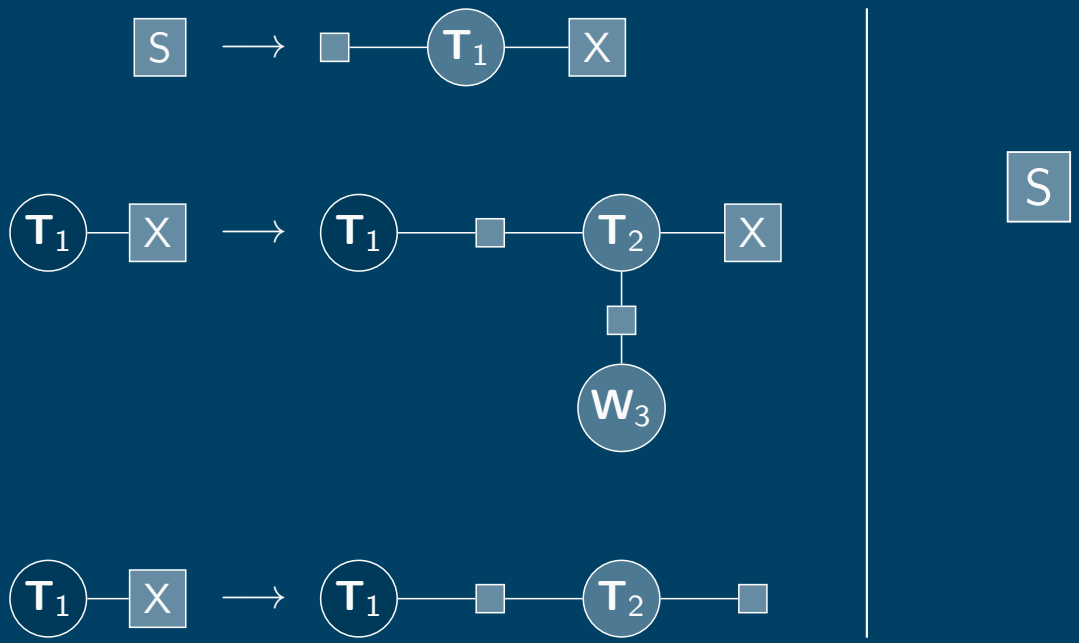

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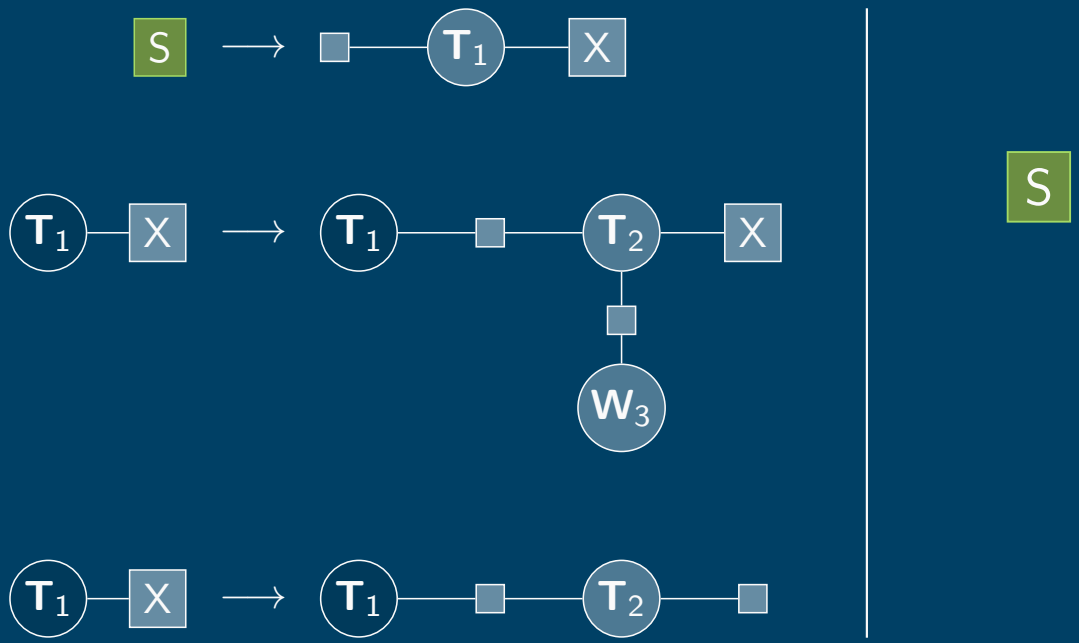

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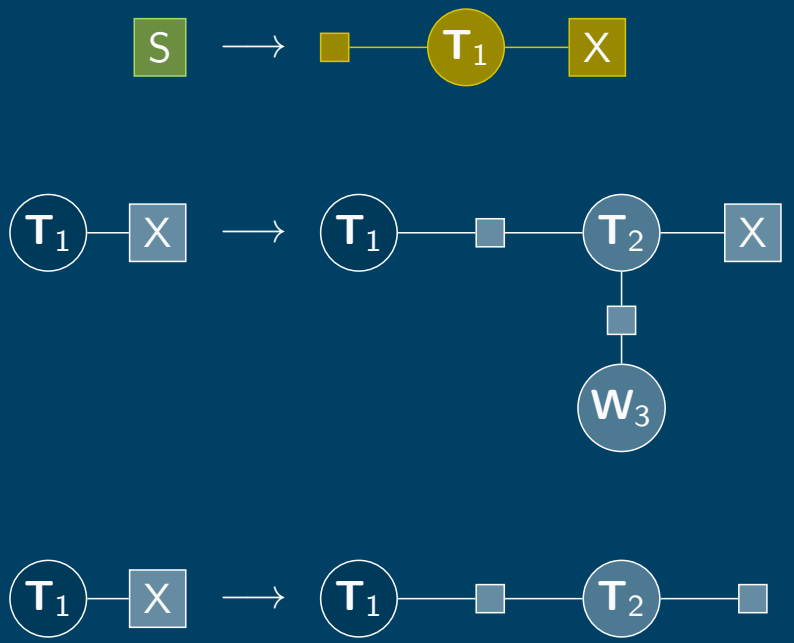

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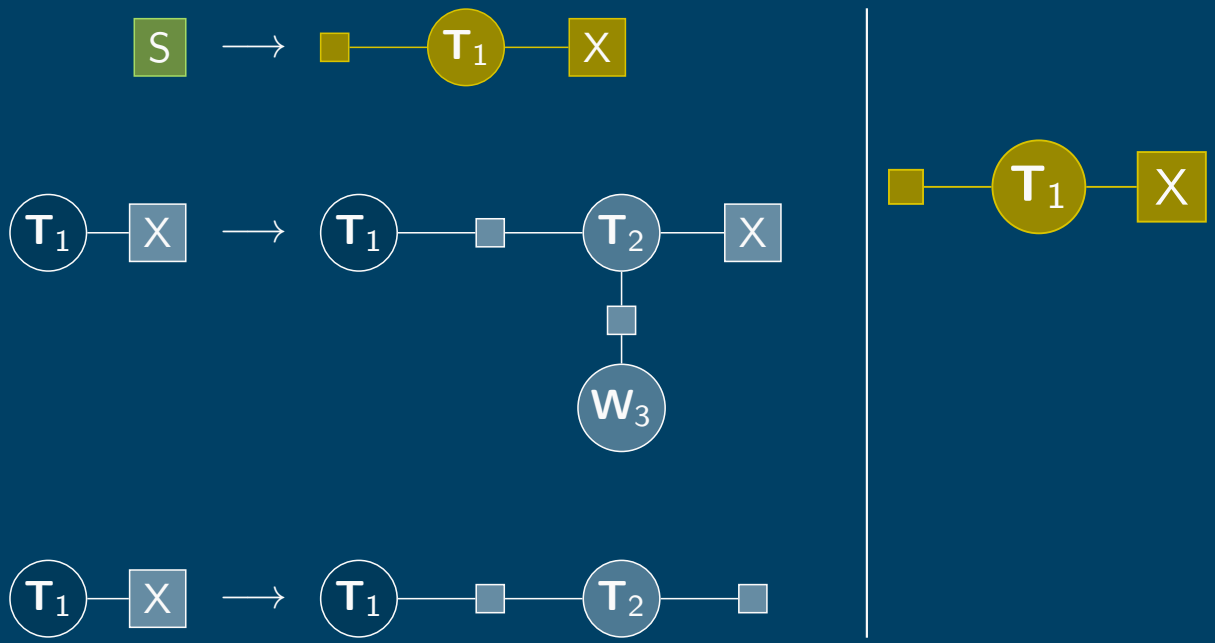

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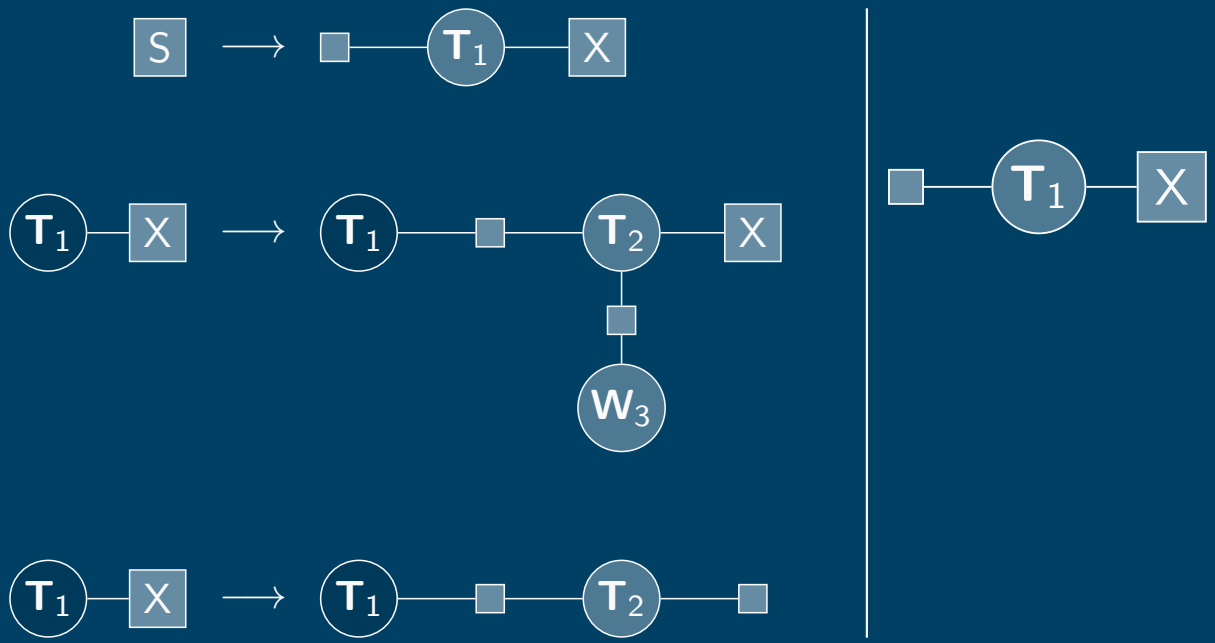

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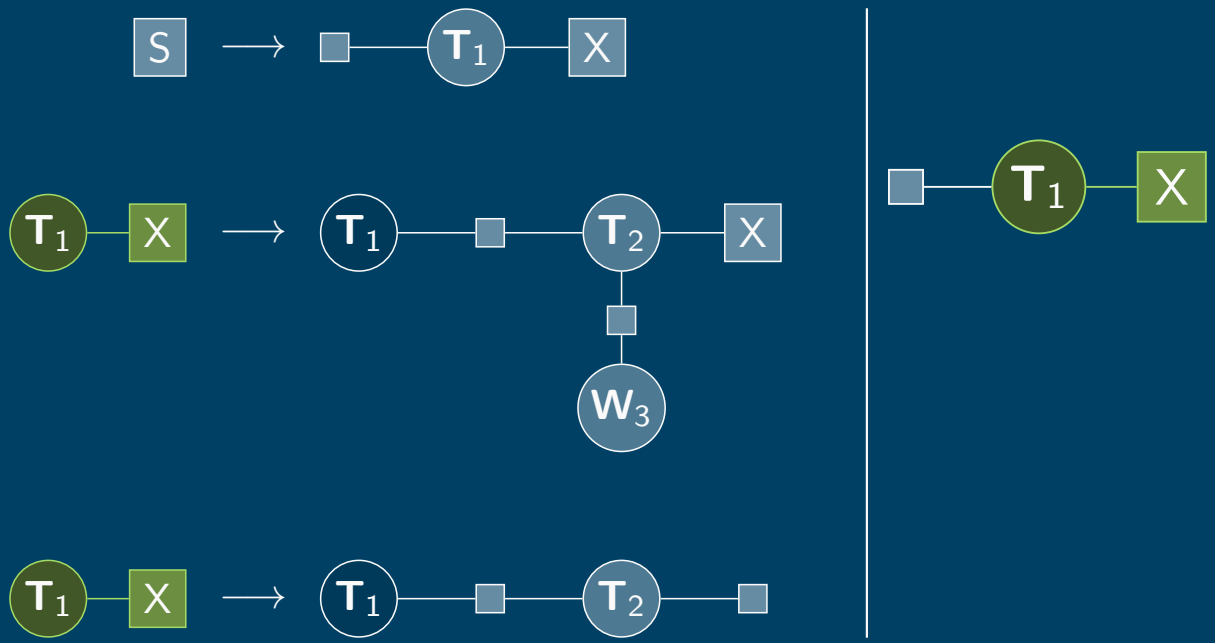

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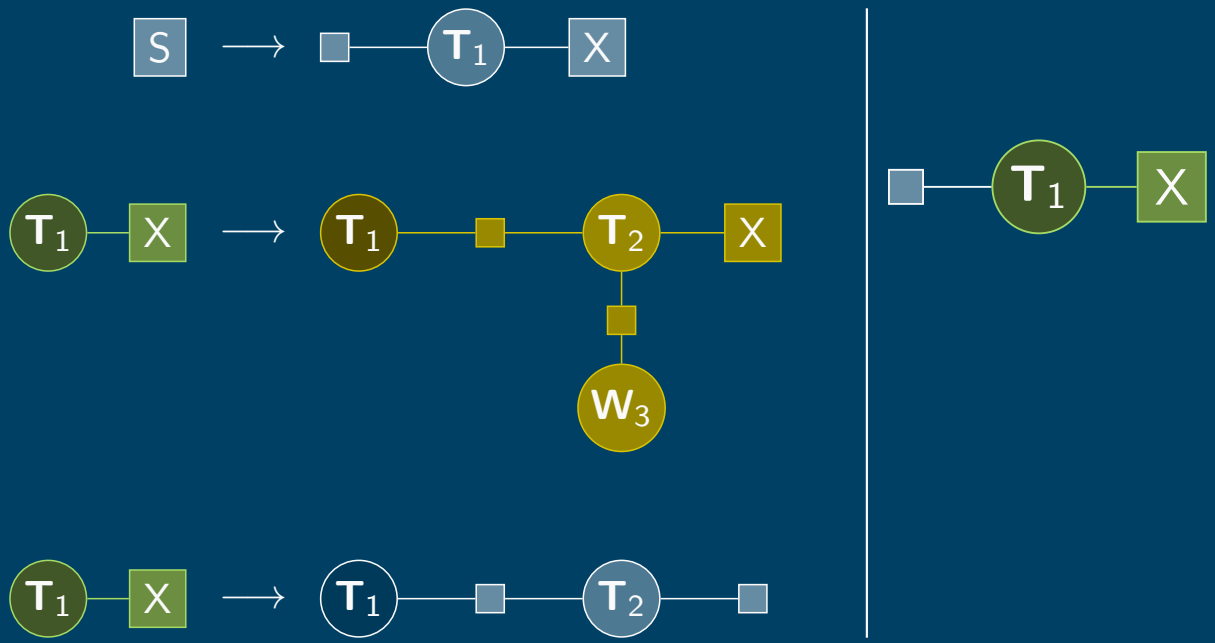

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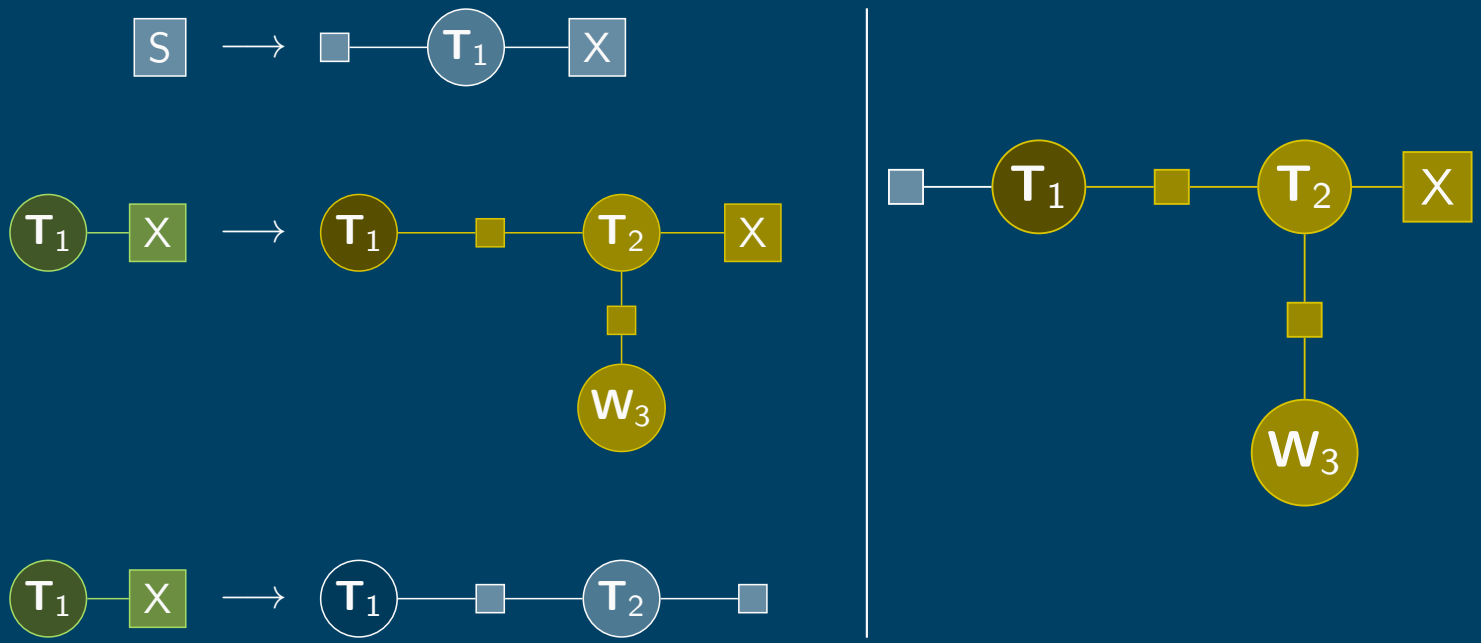

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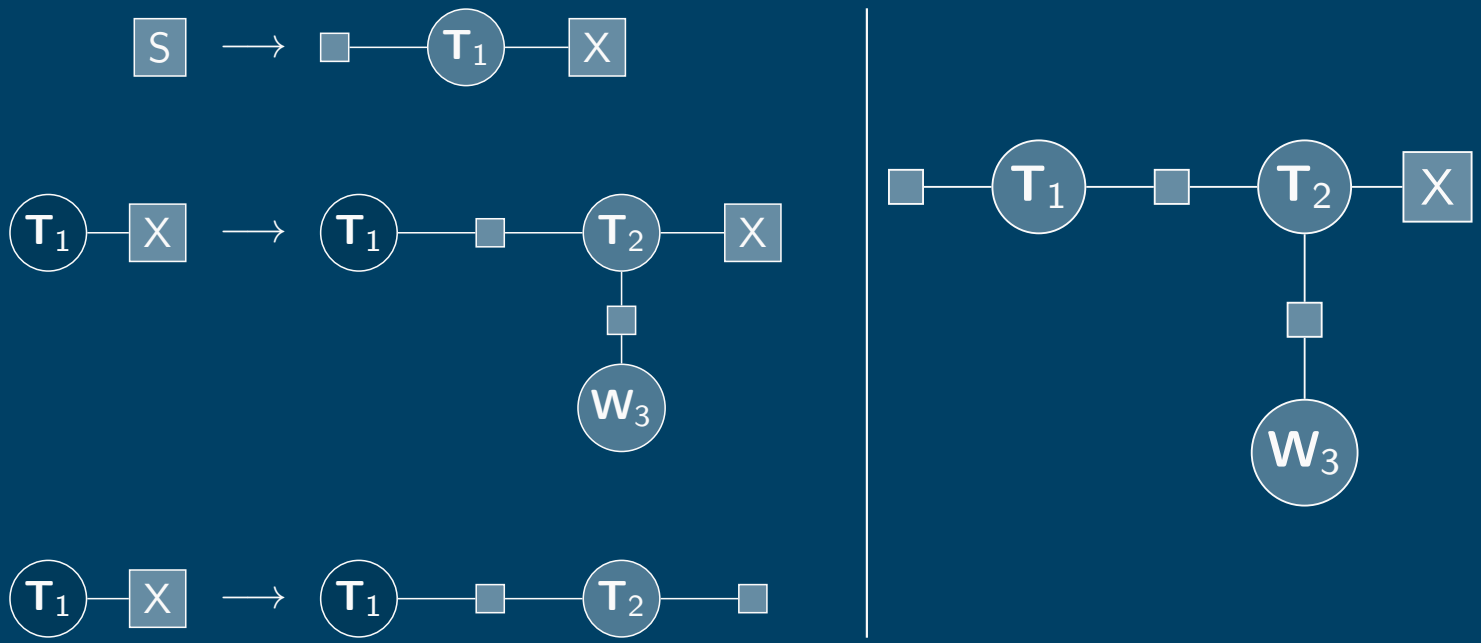

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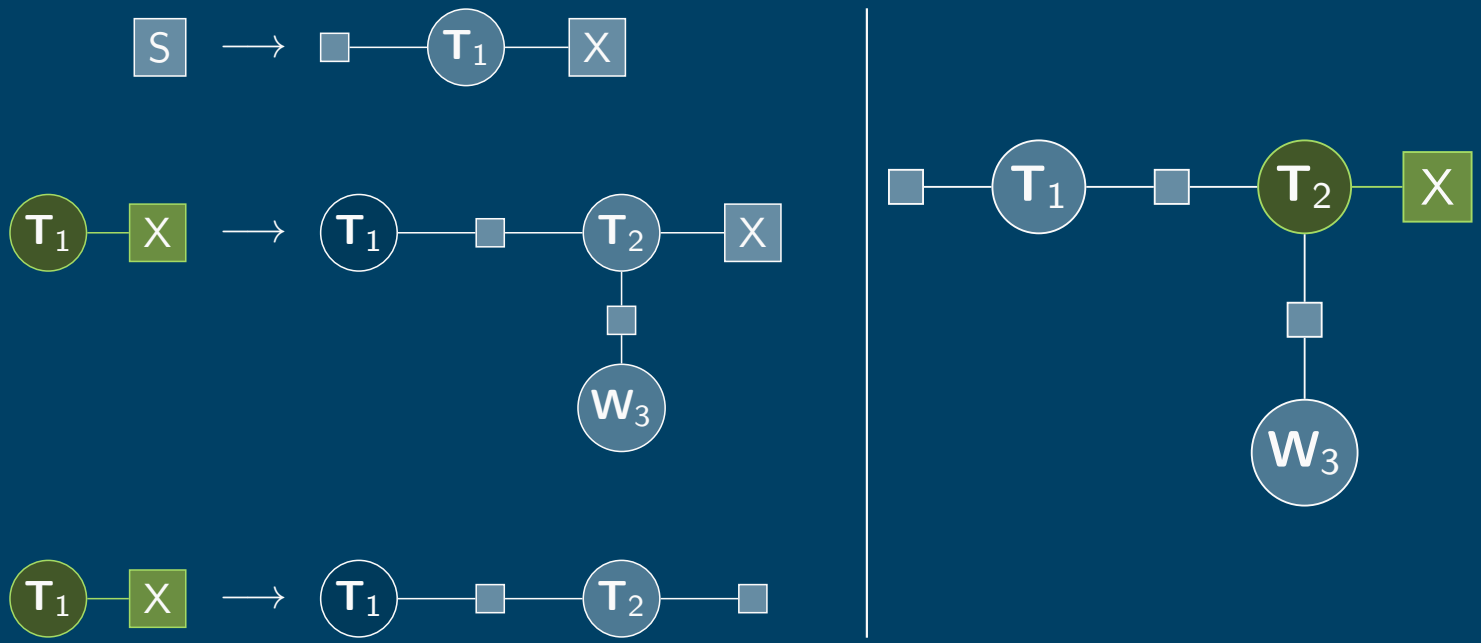

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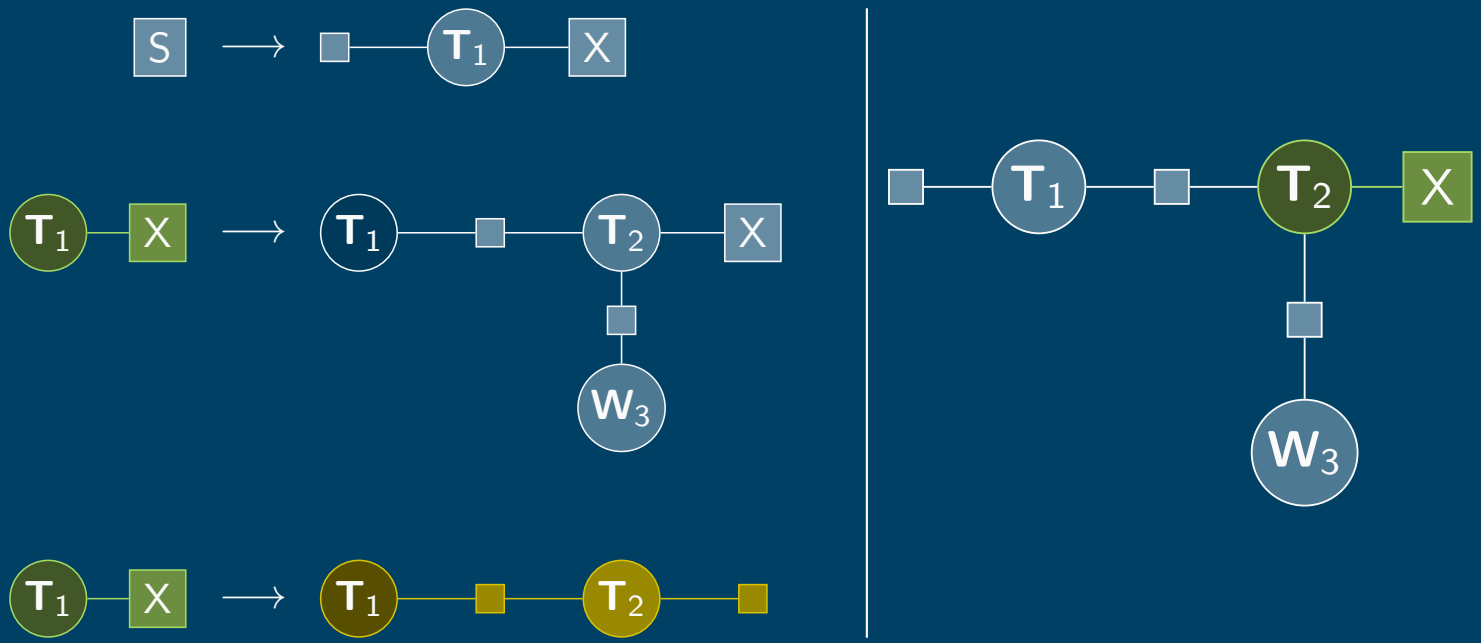

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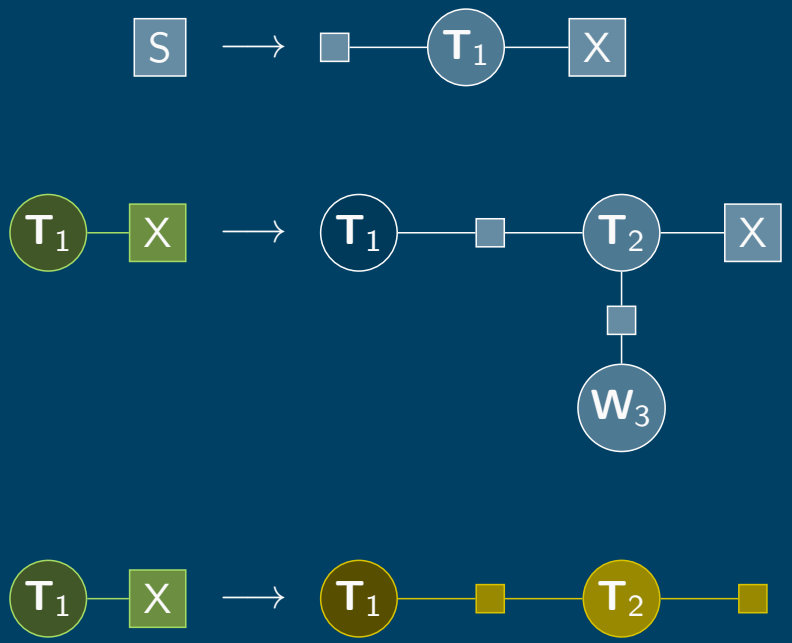

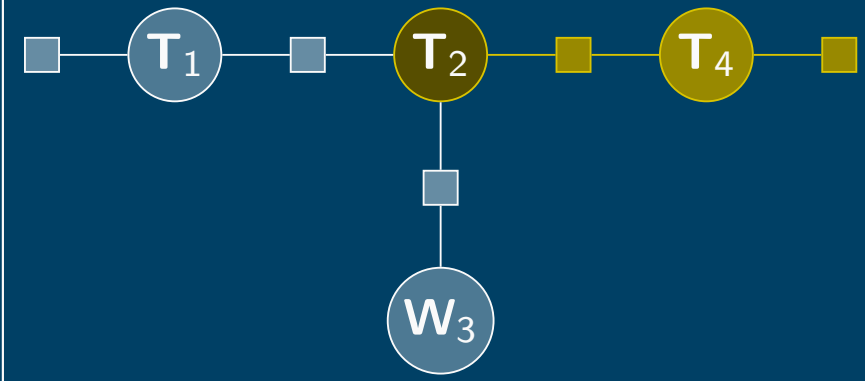

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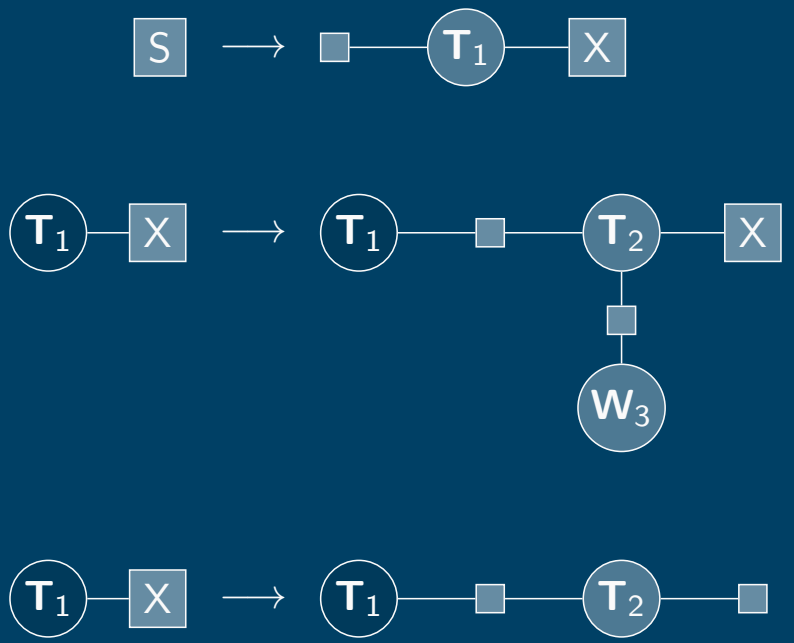

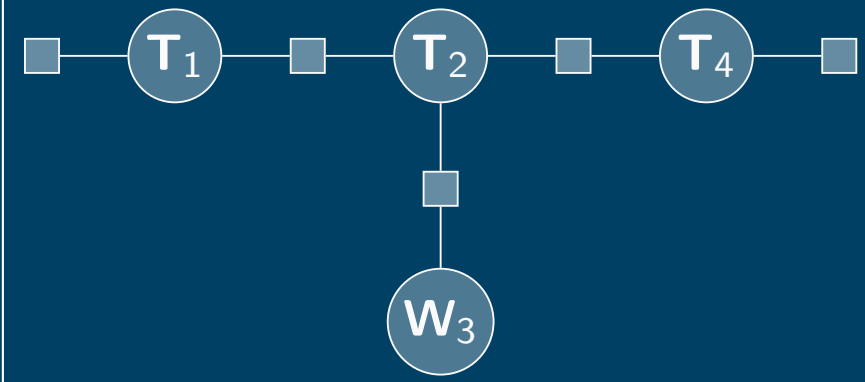

A Factor Graph Grammar for PCFGs

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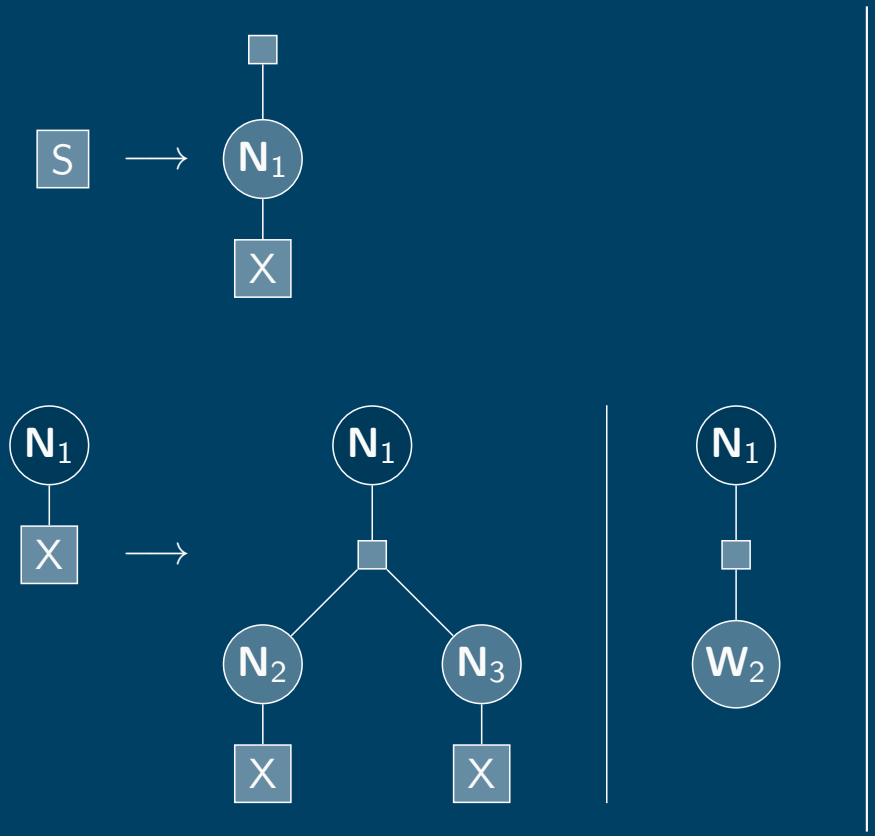

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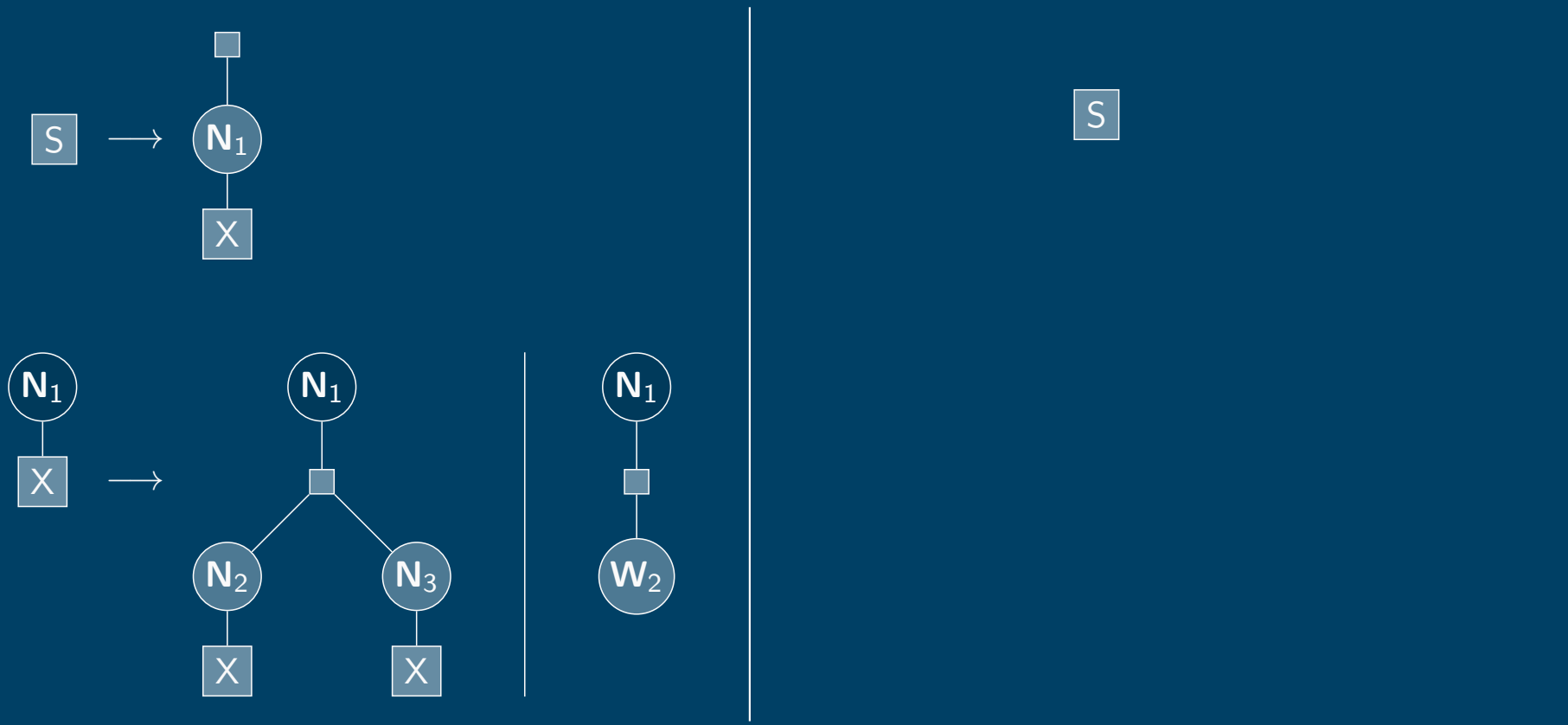

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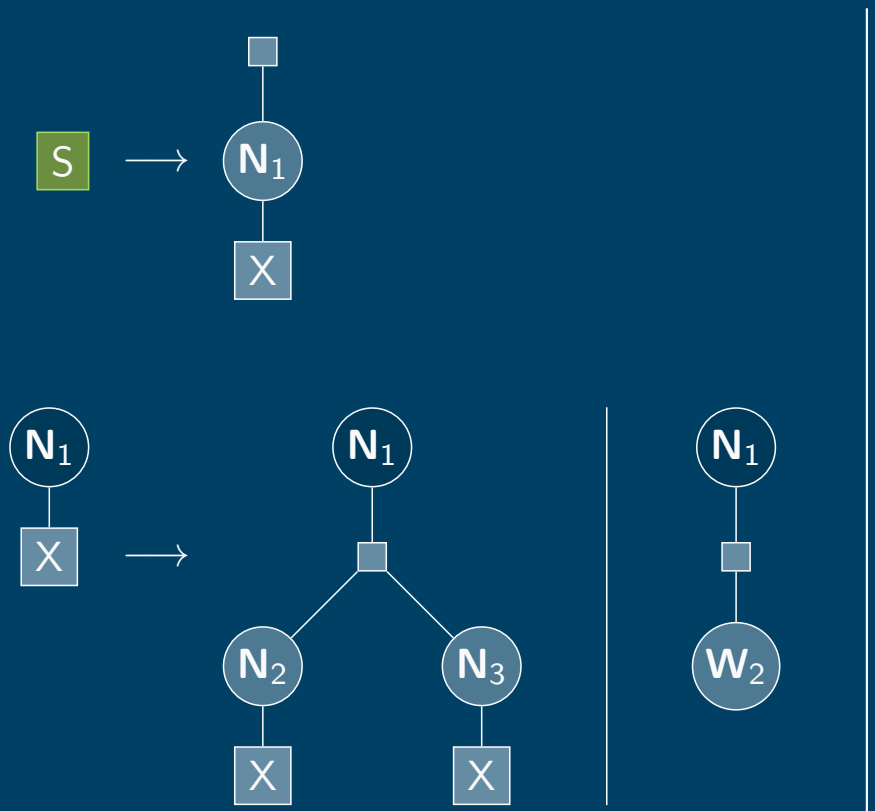

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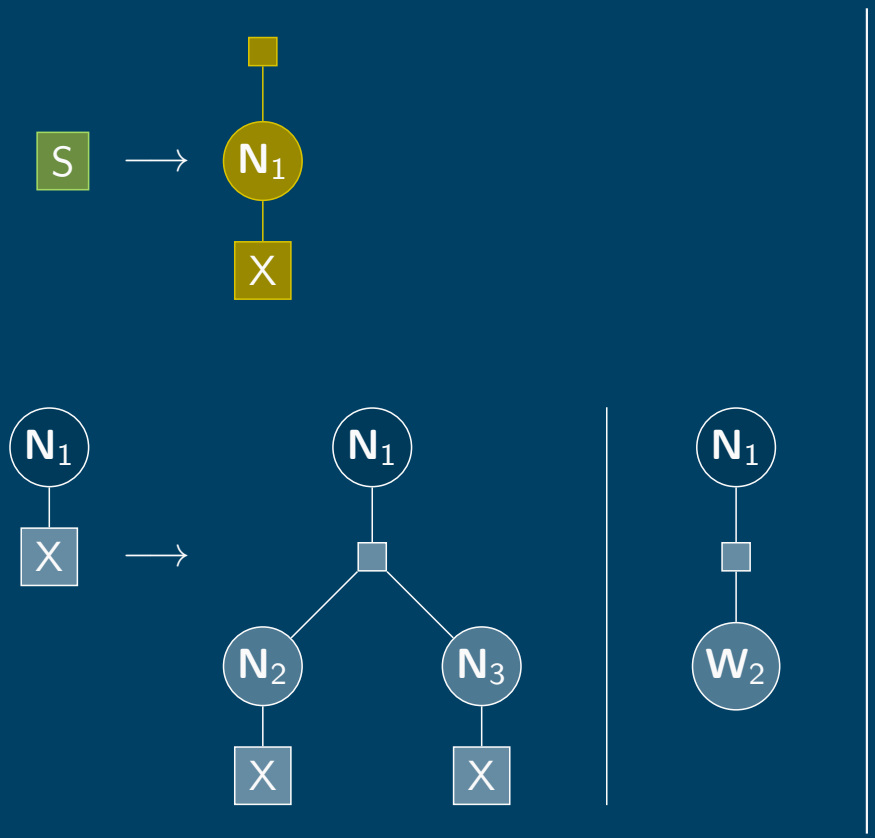

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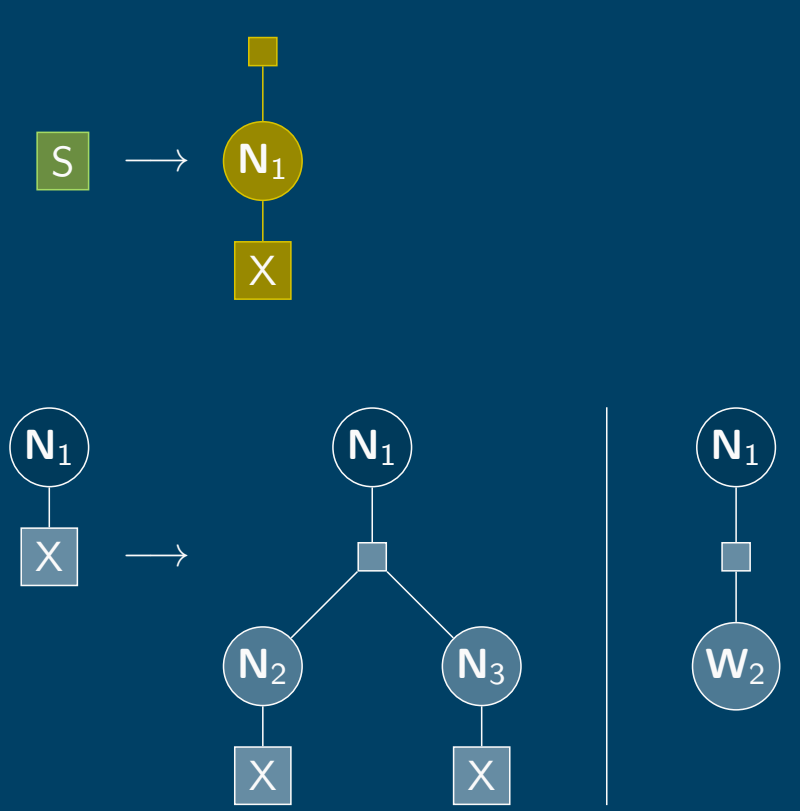

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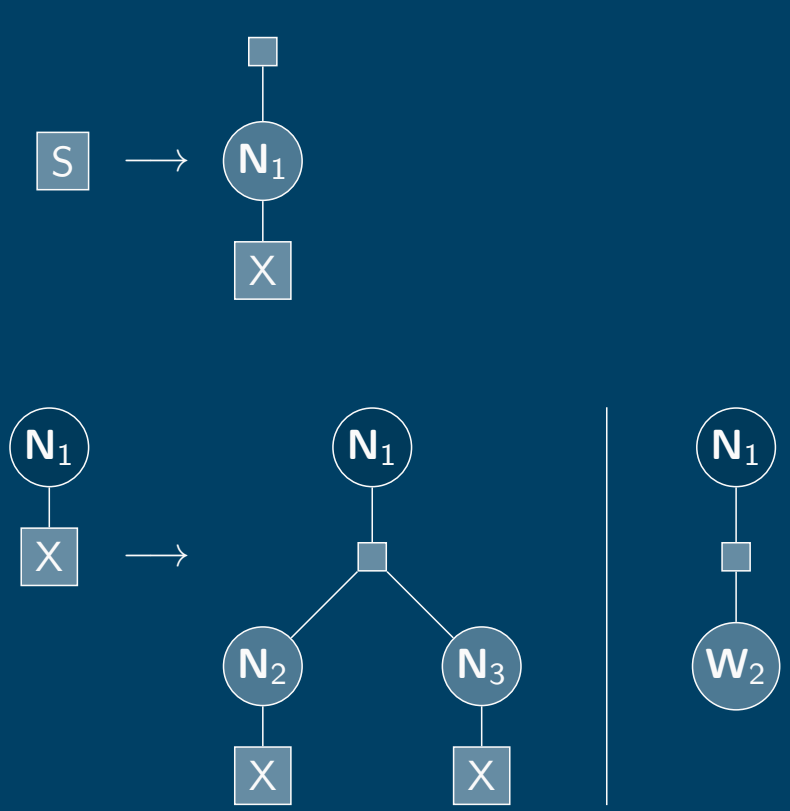

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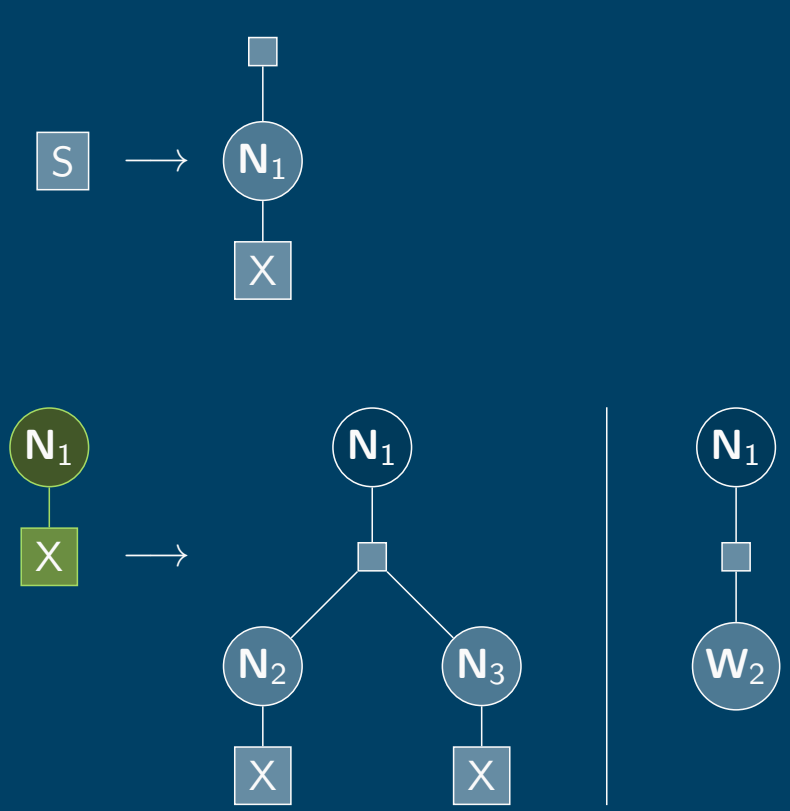

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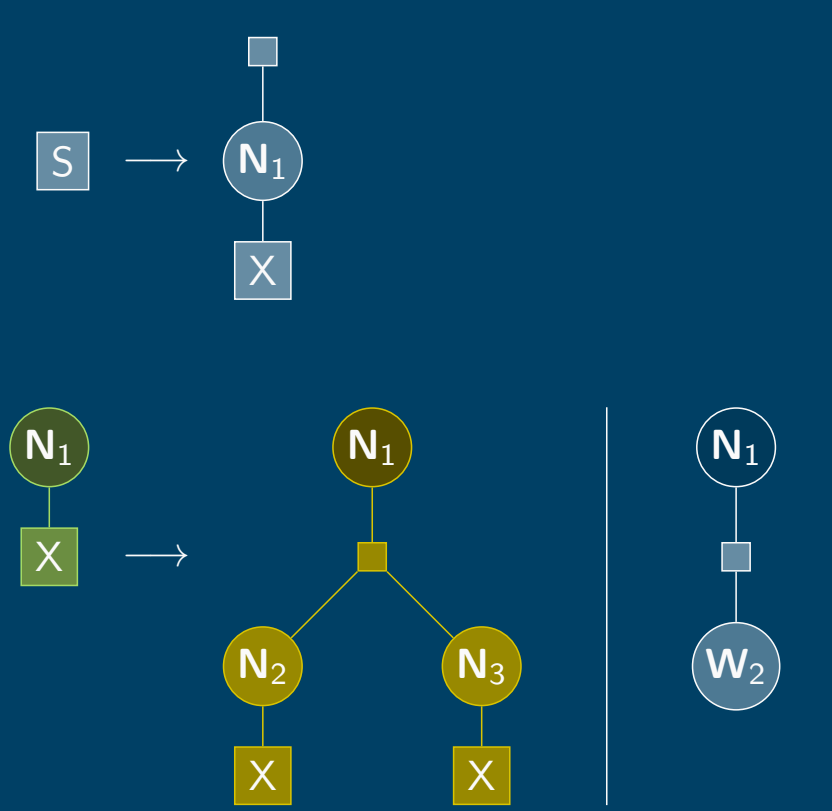

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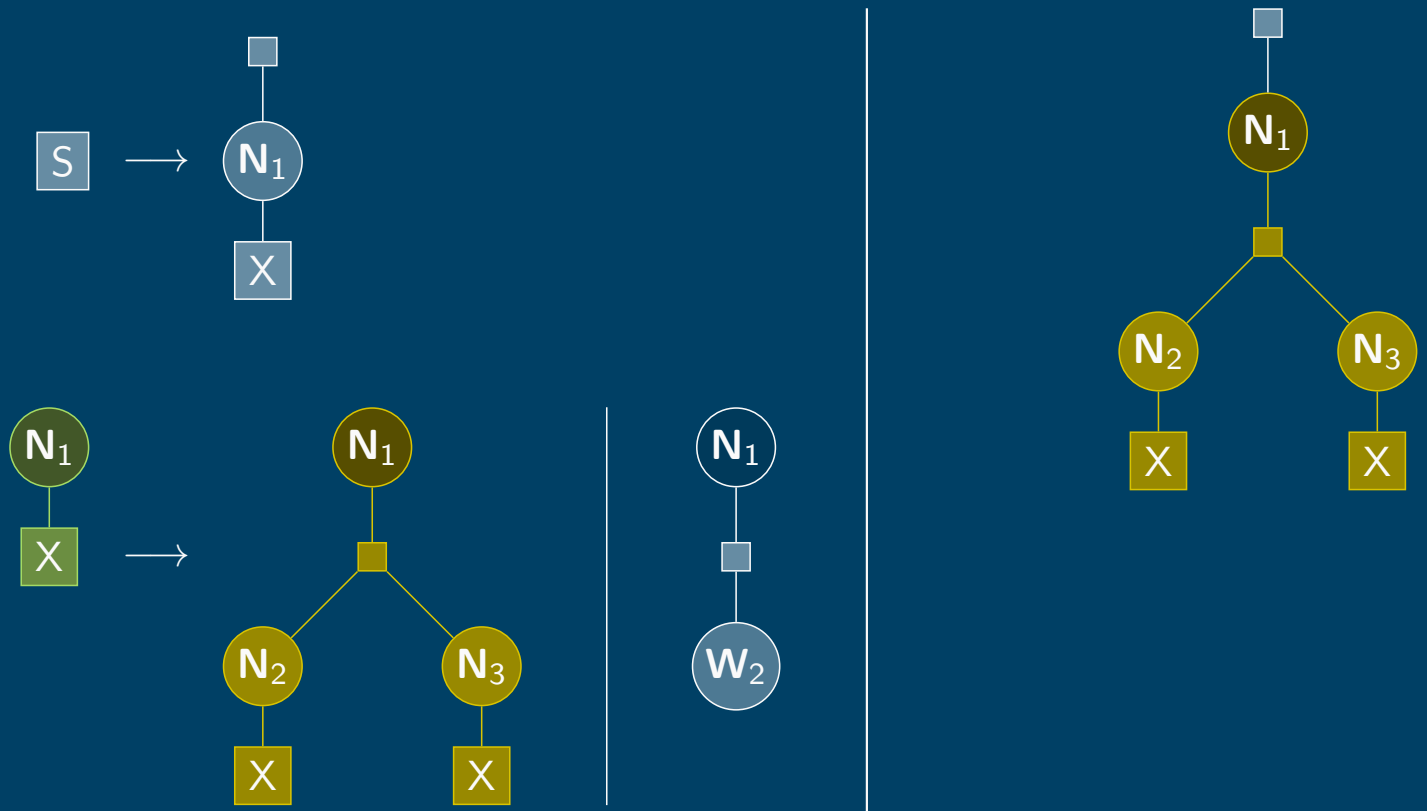
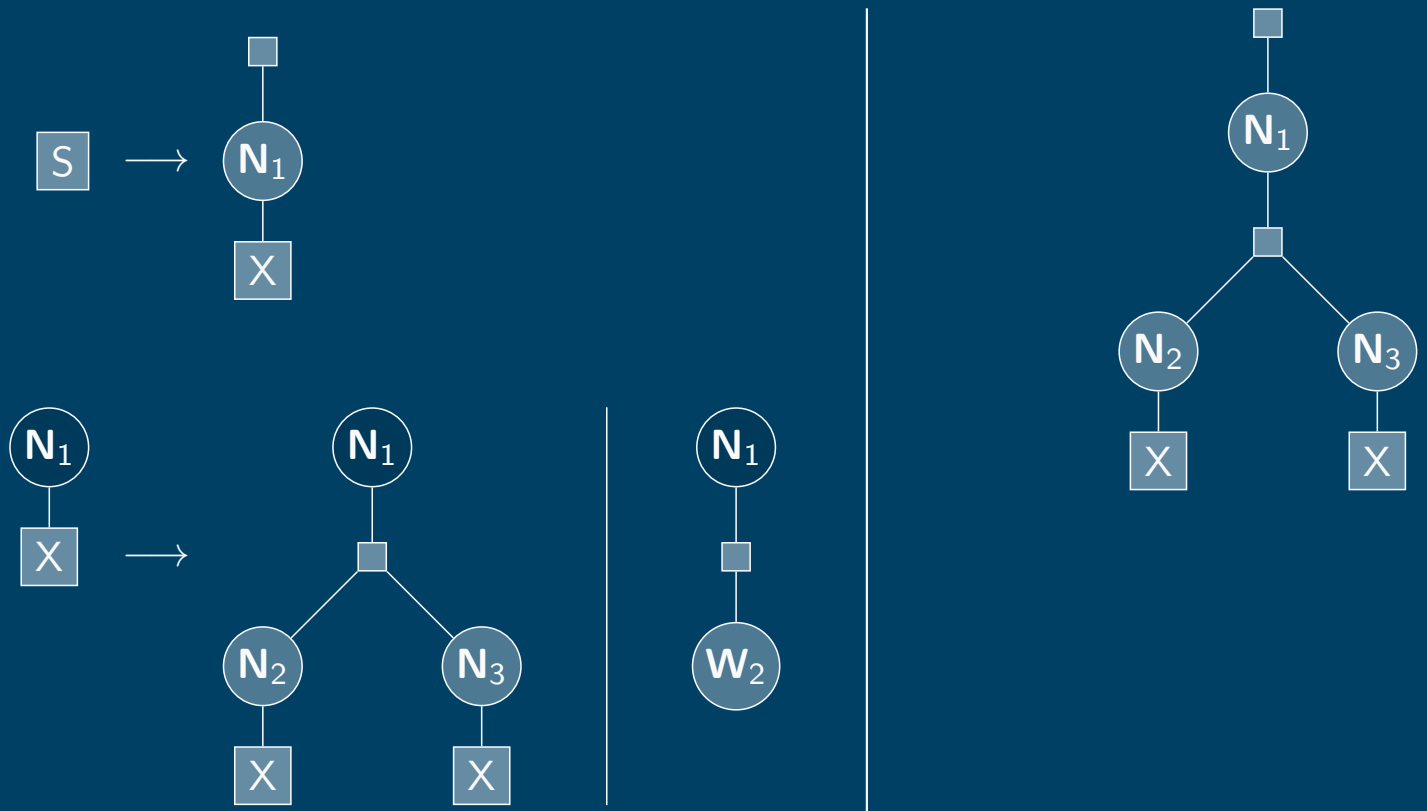


A Factor Graph Grammar for PCFGs



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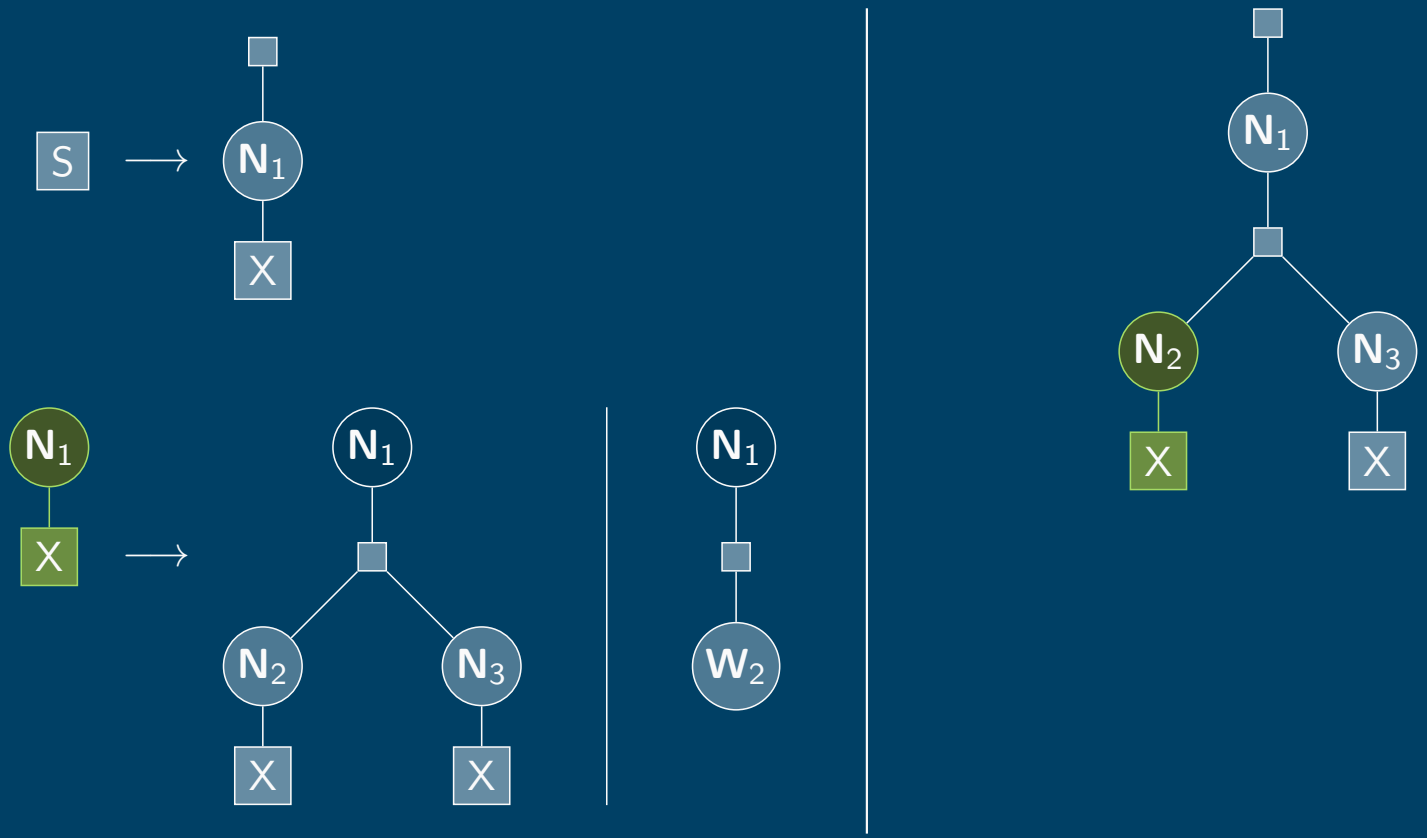

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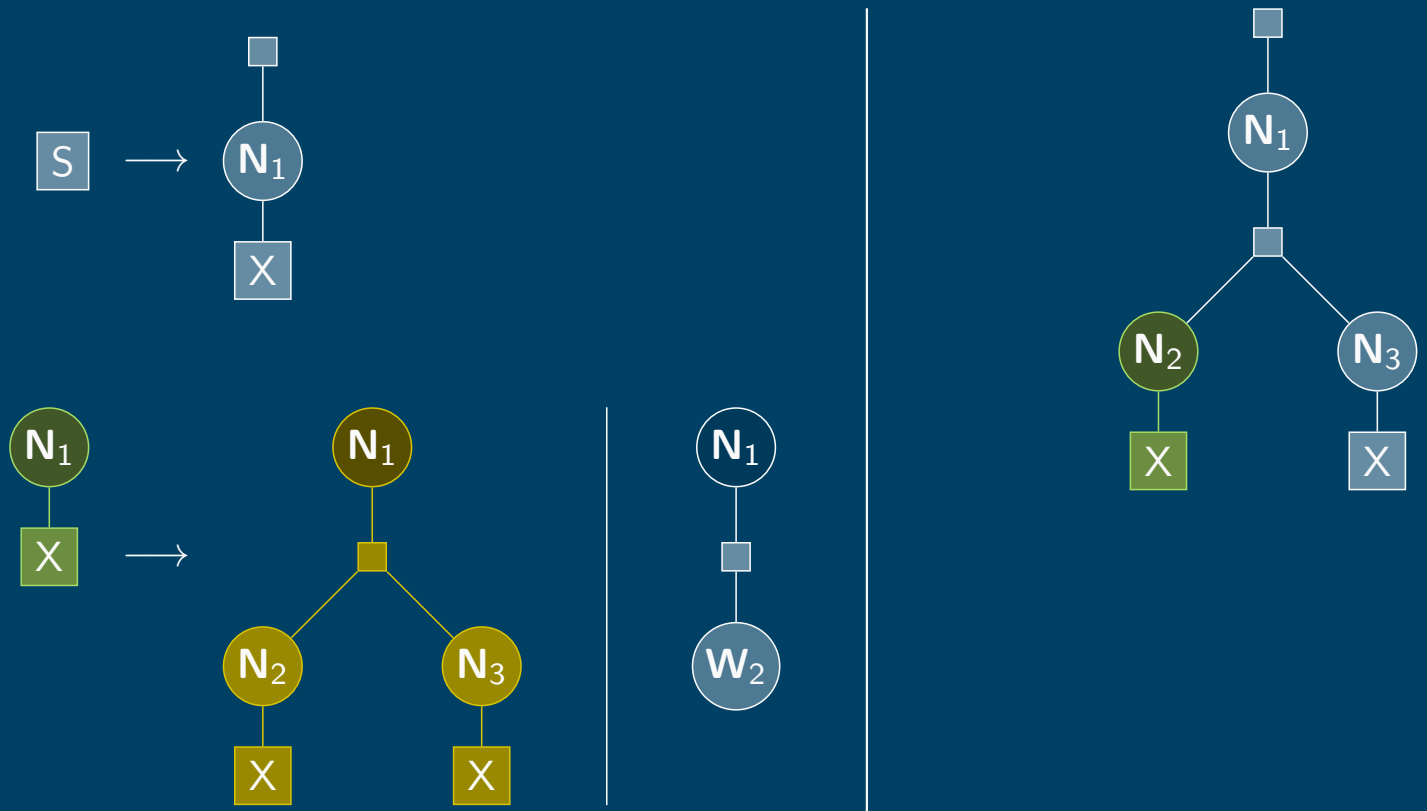

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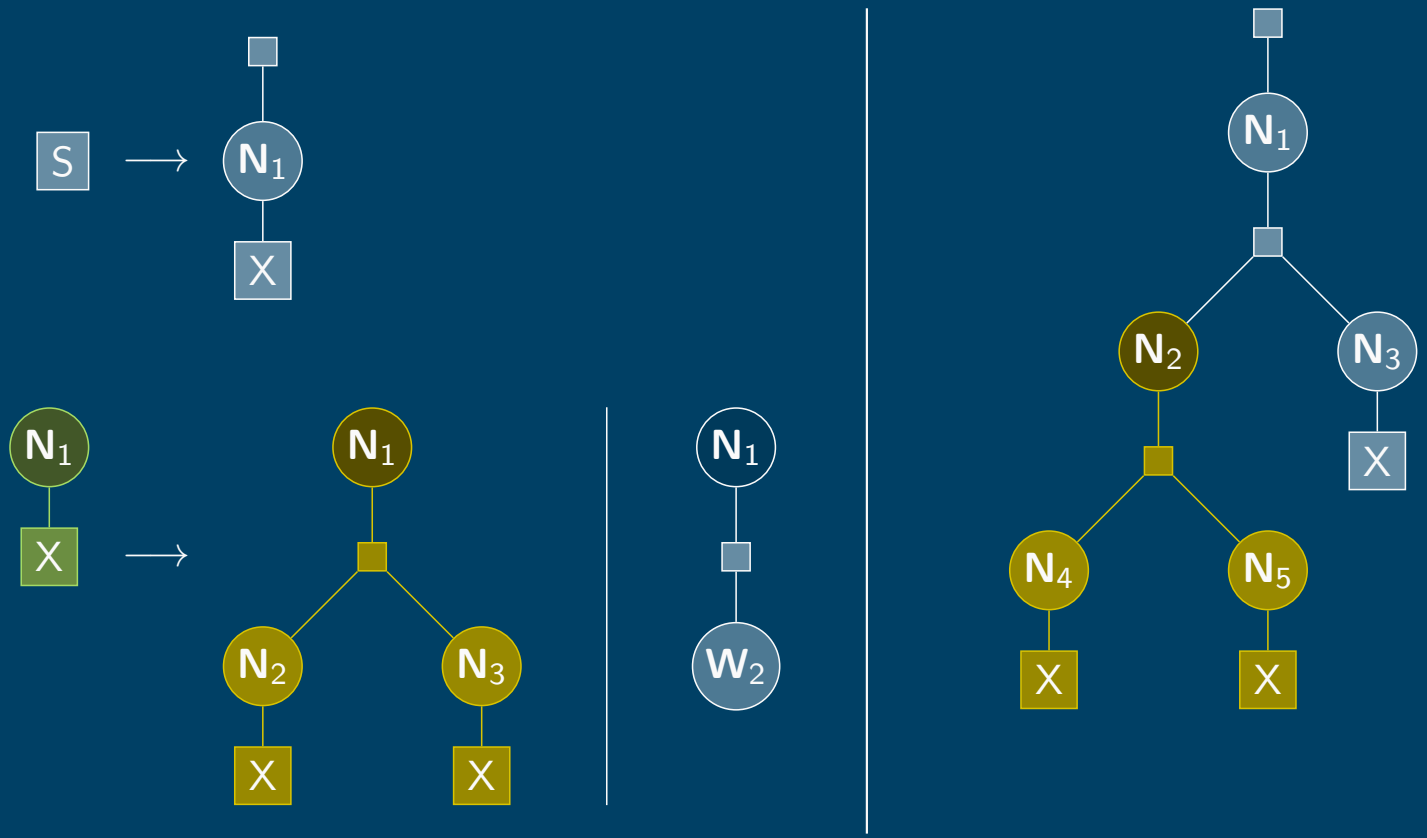

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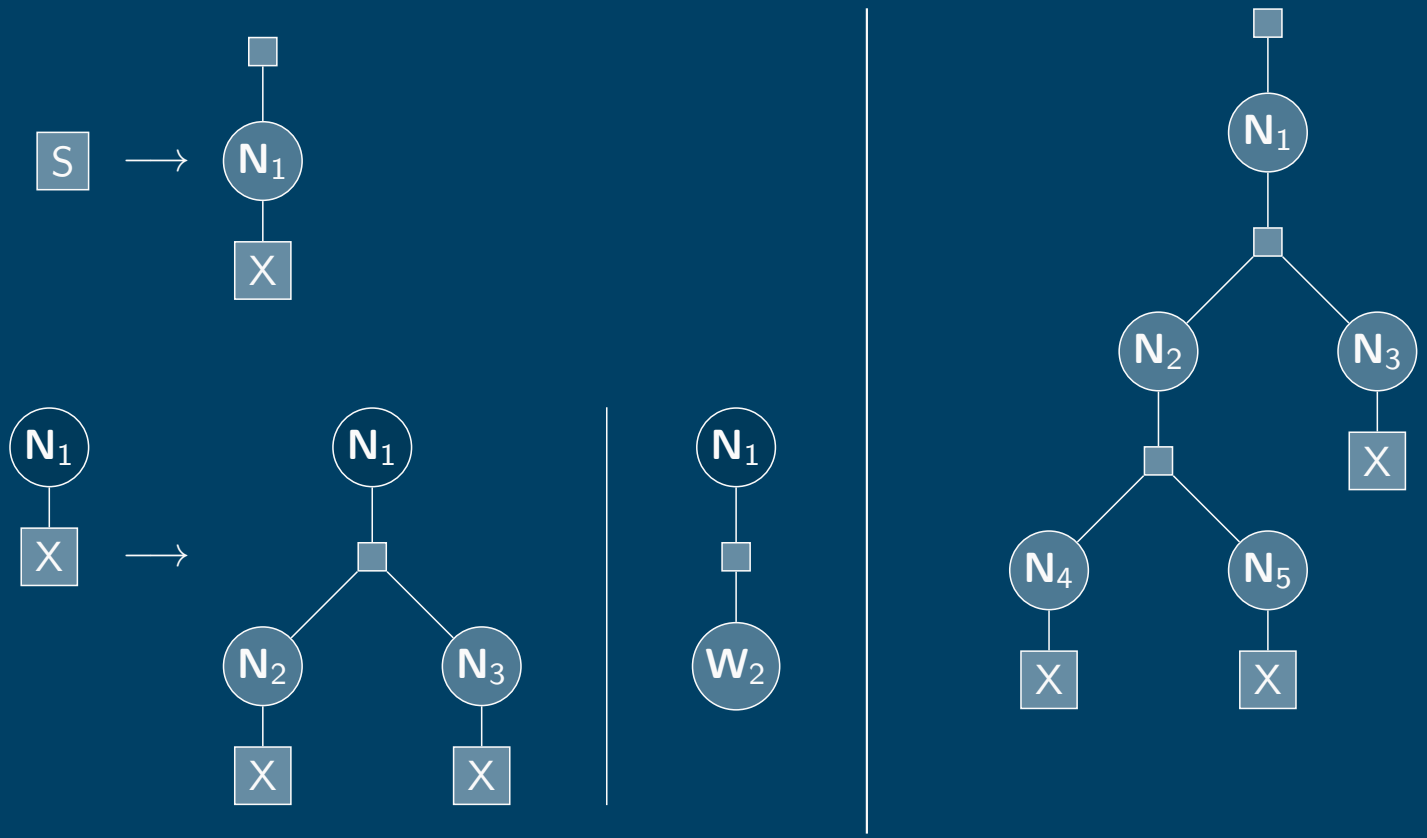

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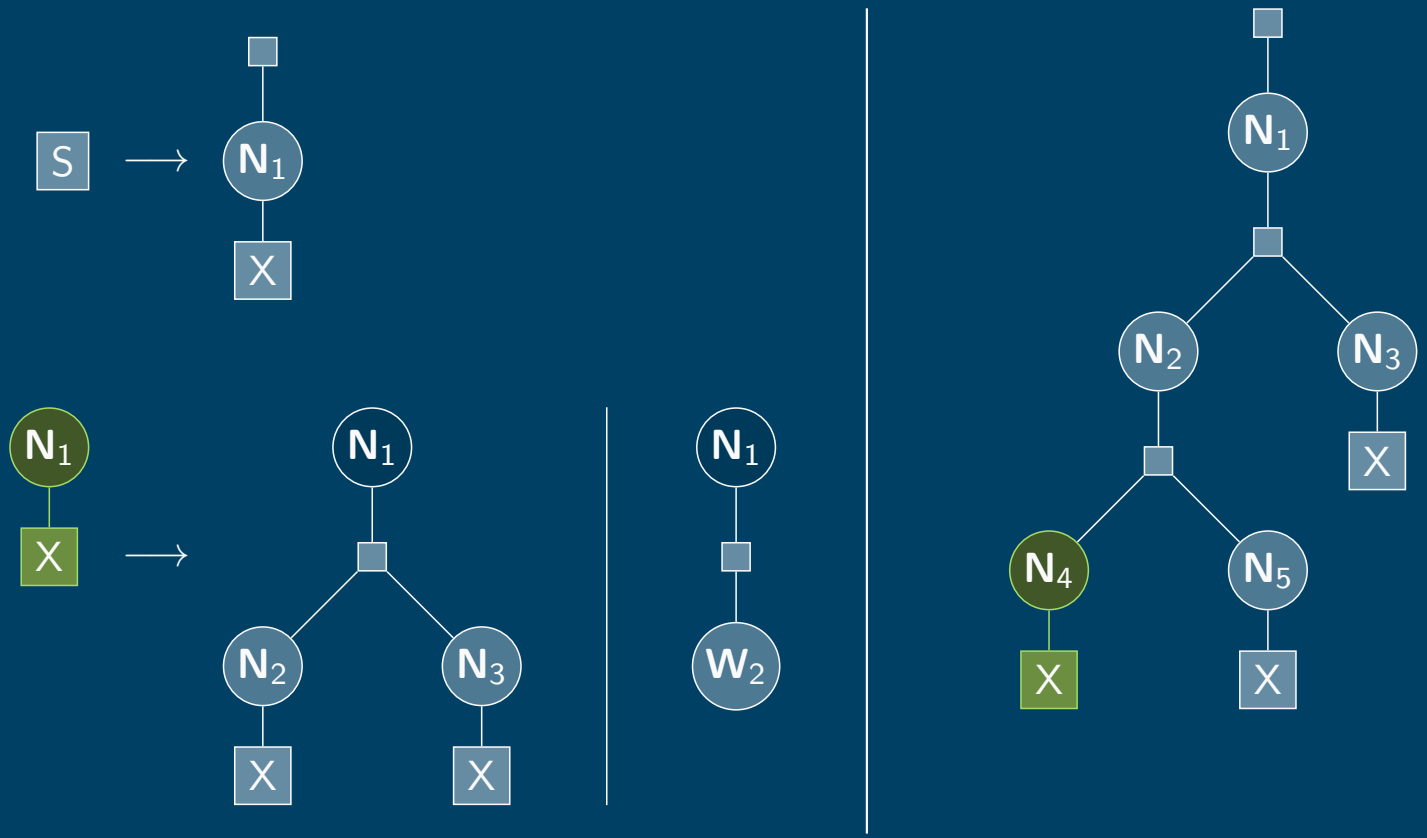

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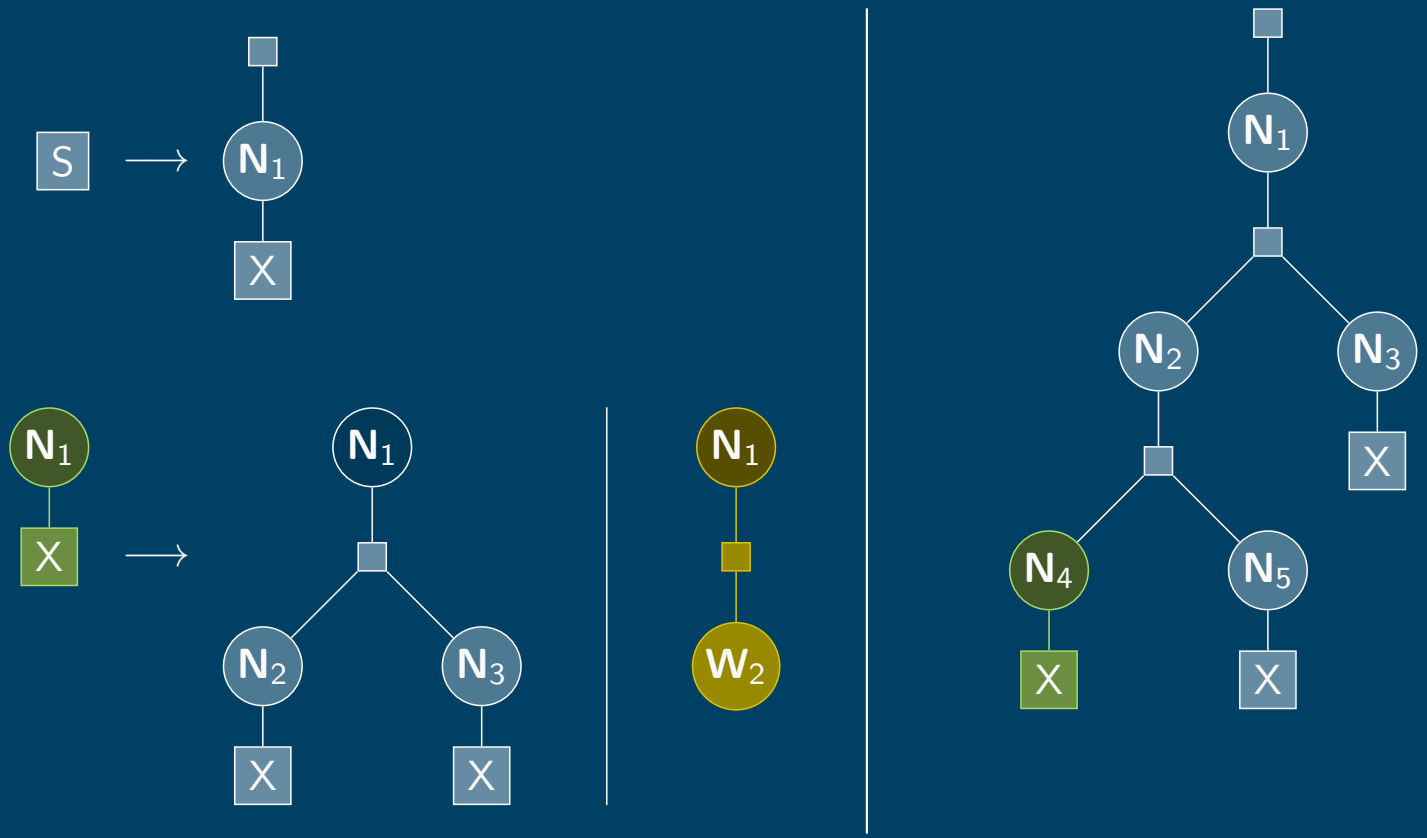

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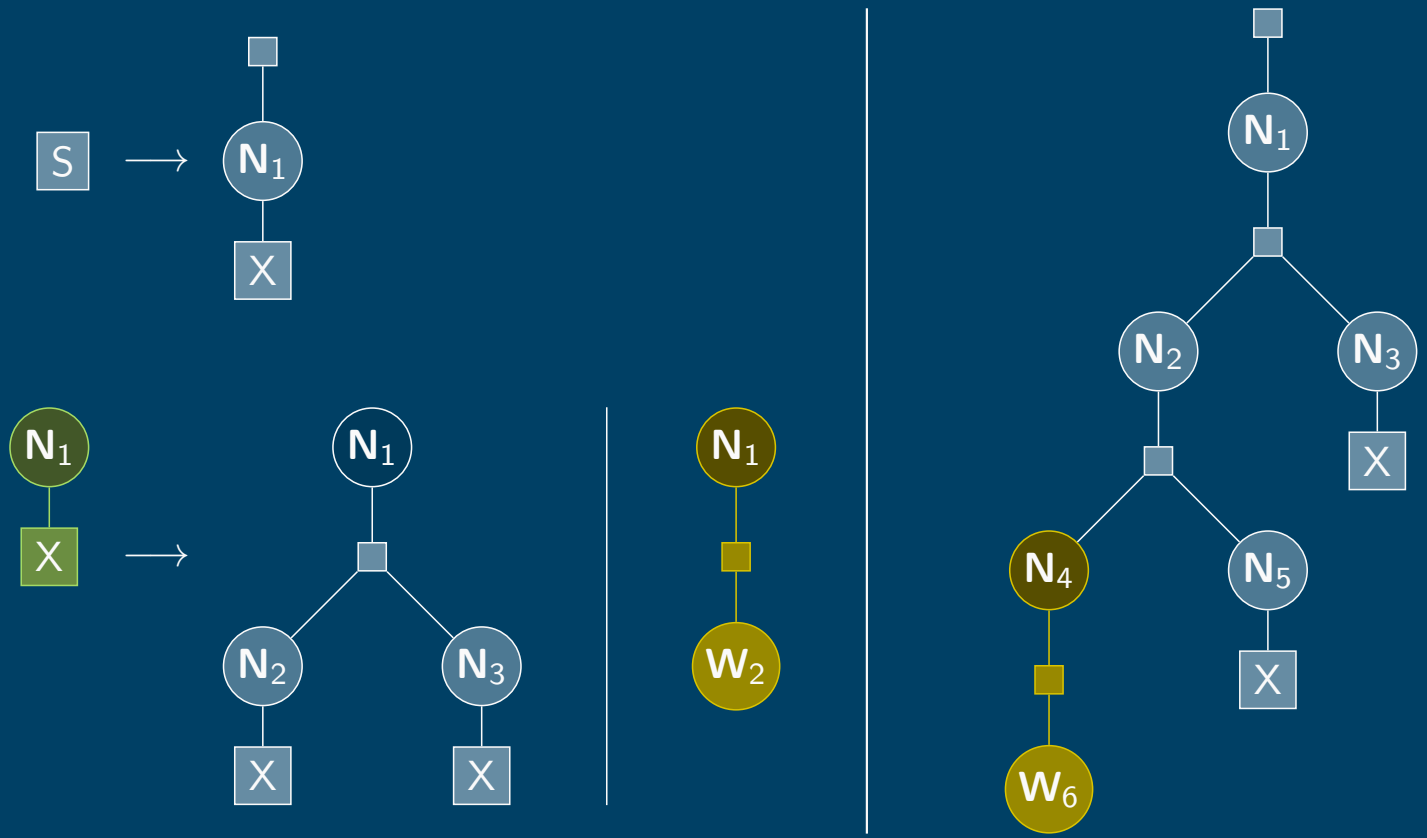

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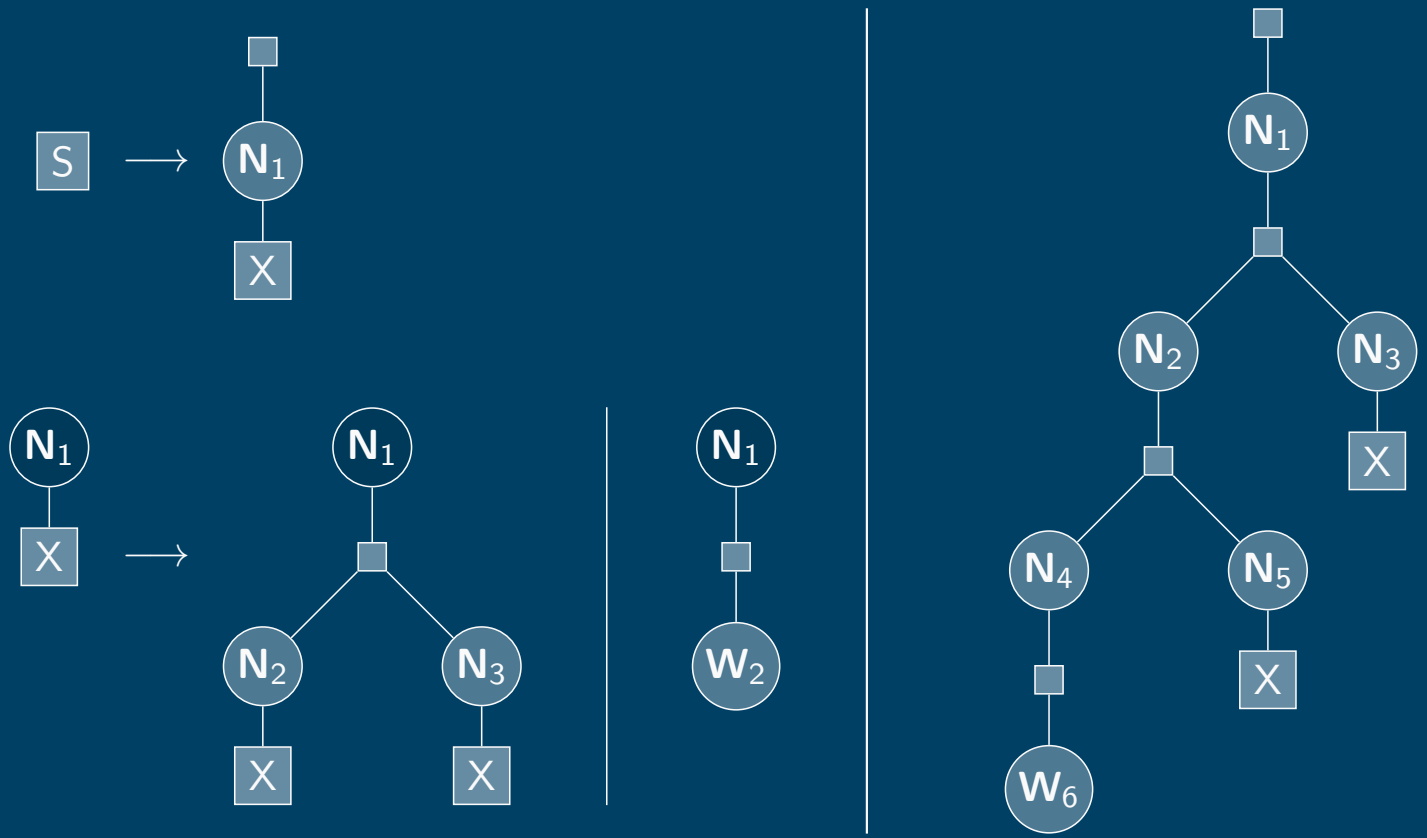

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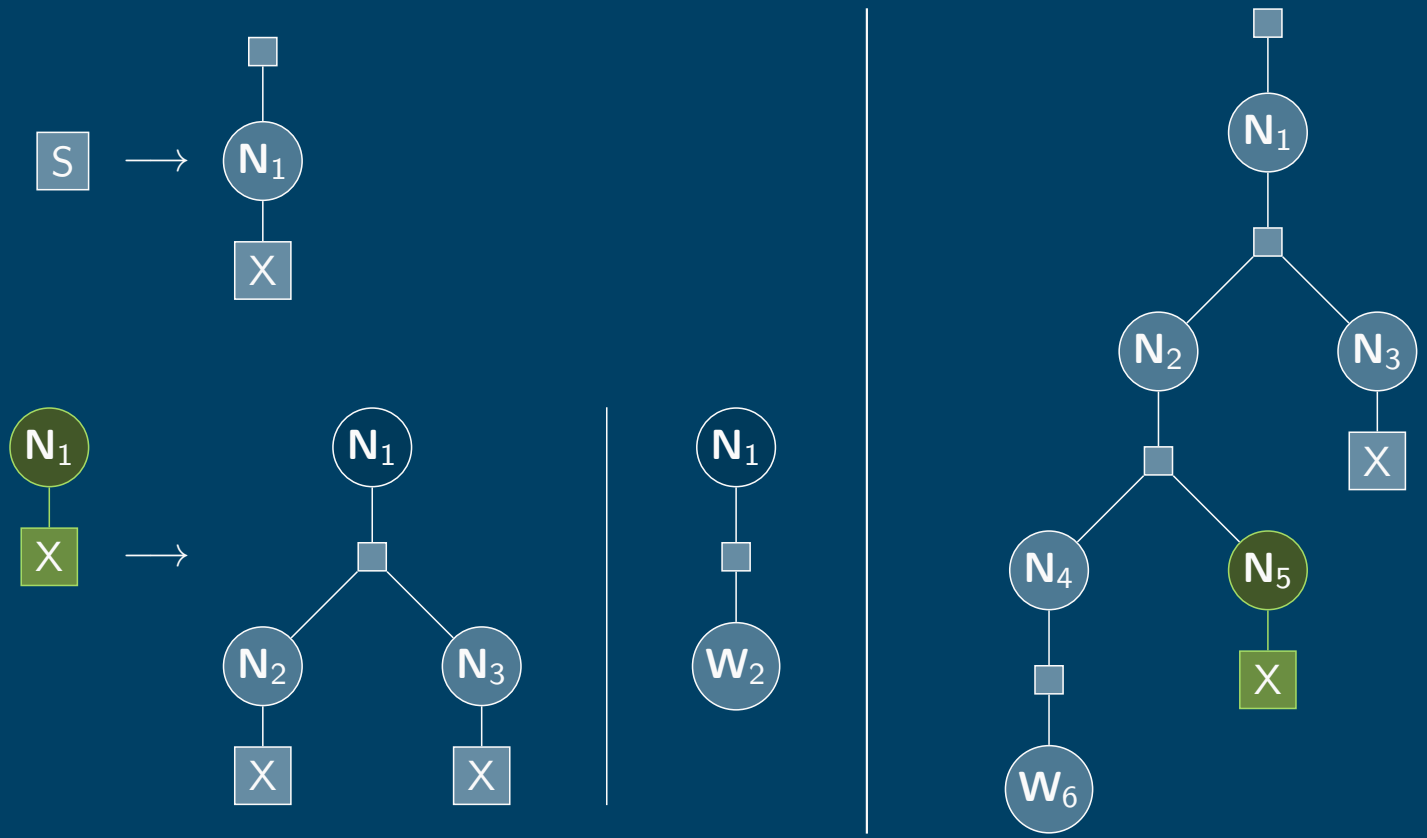

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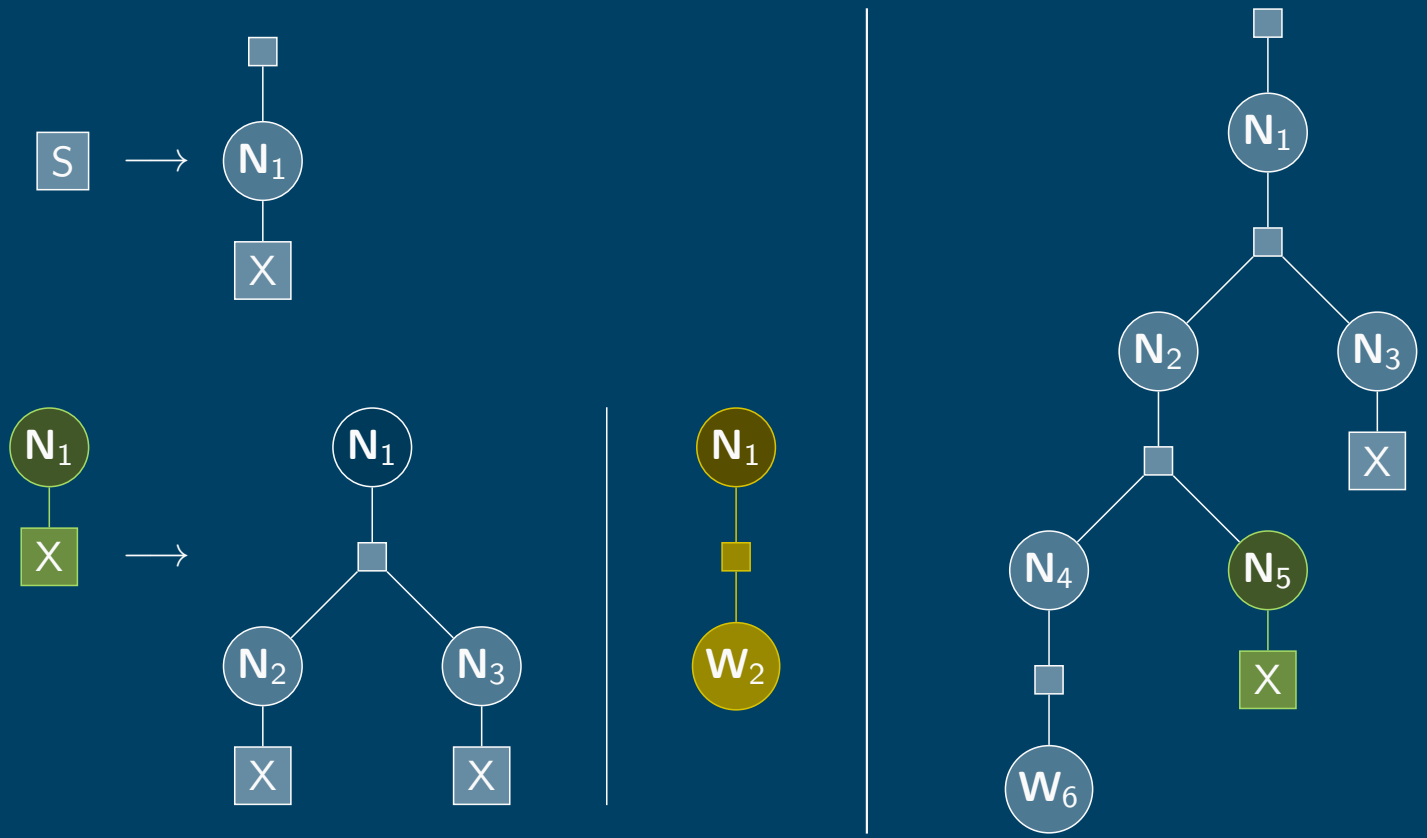

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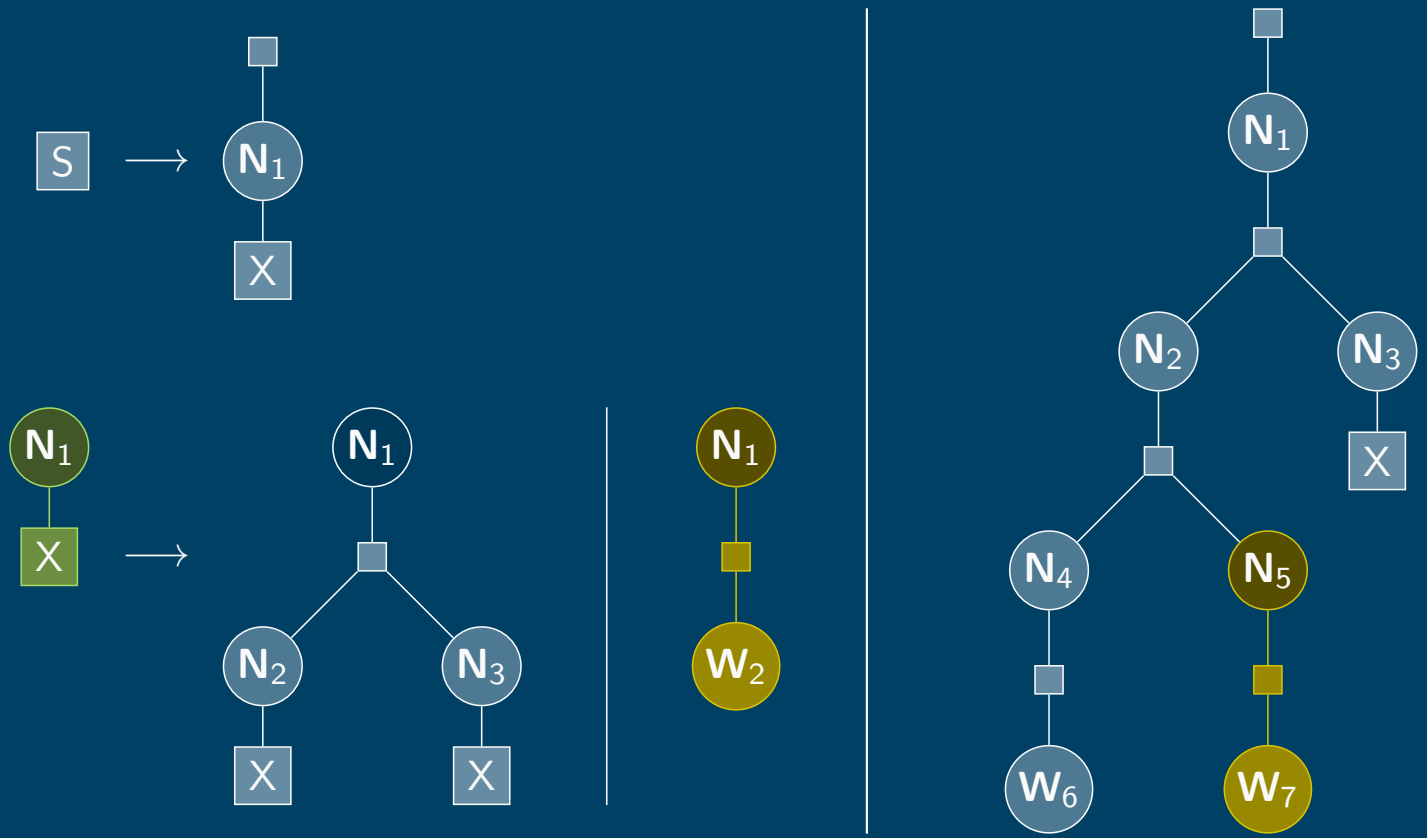

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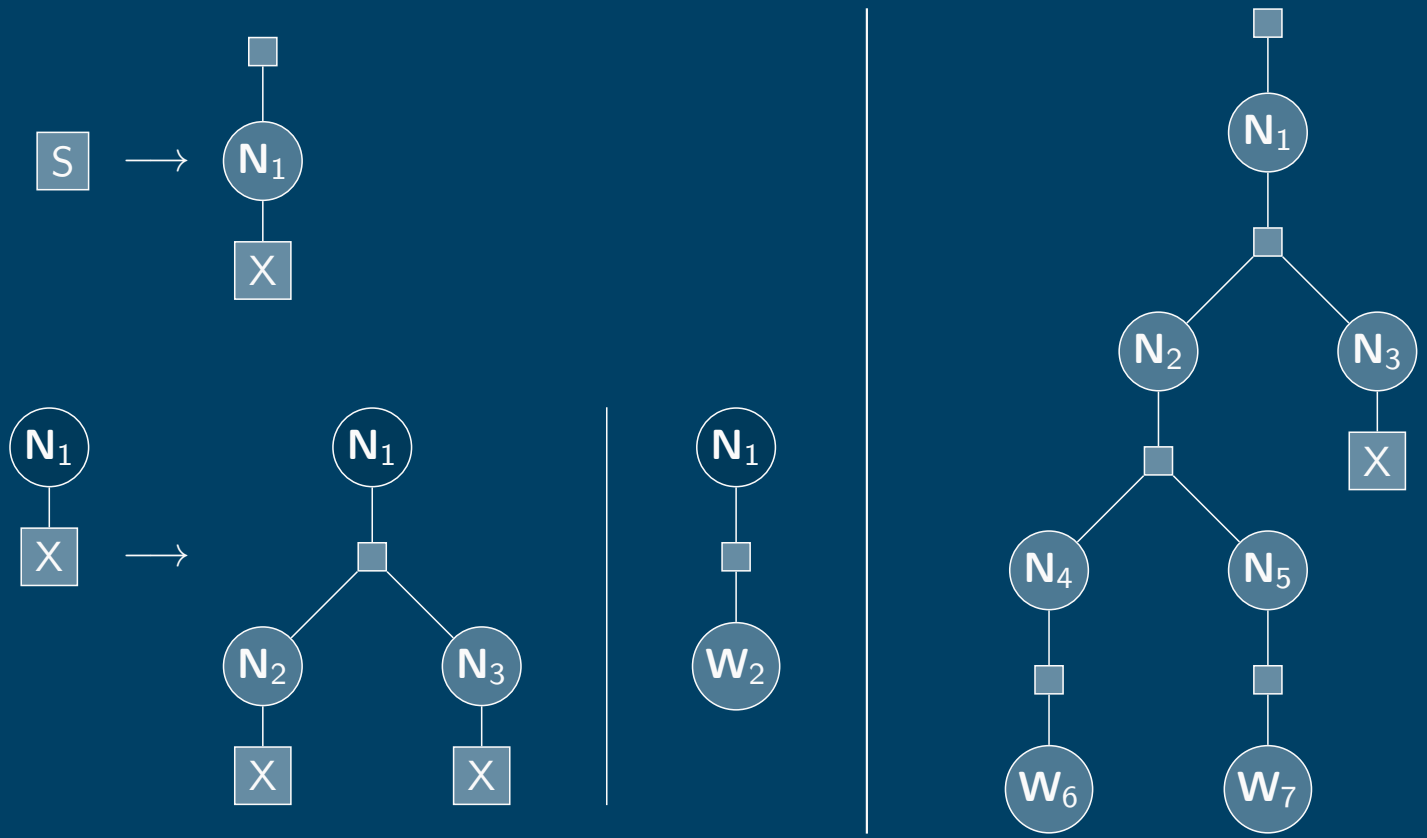

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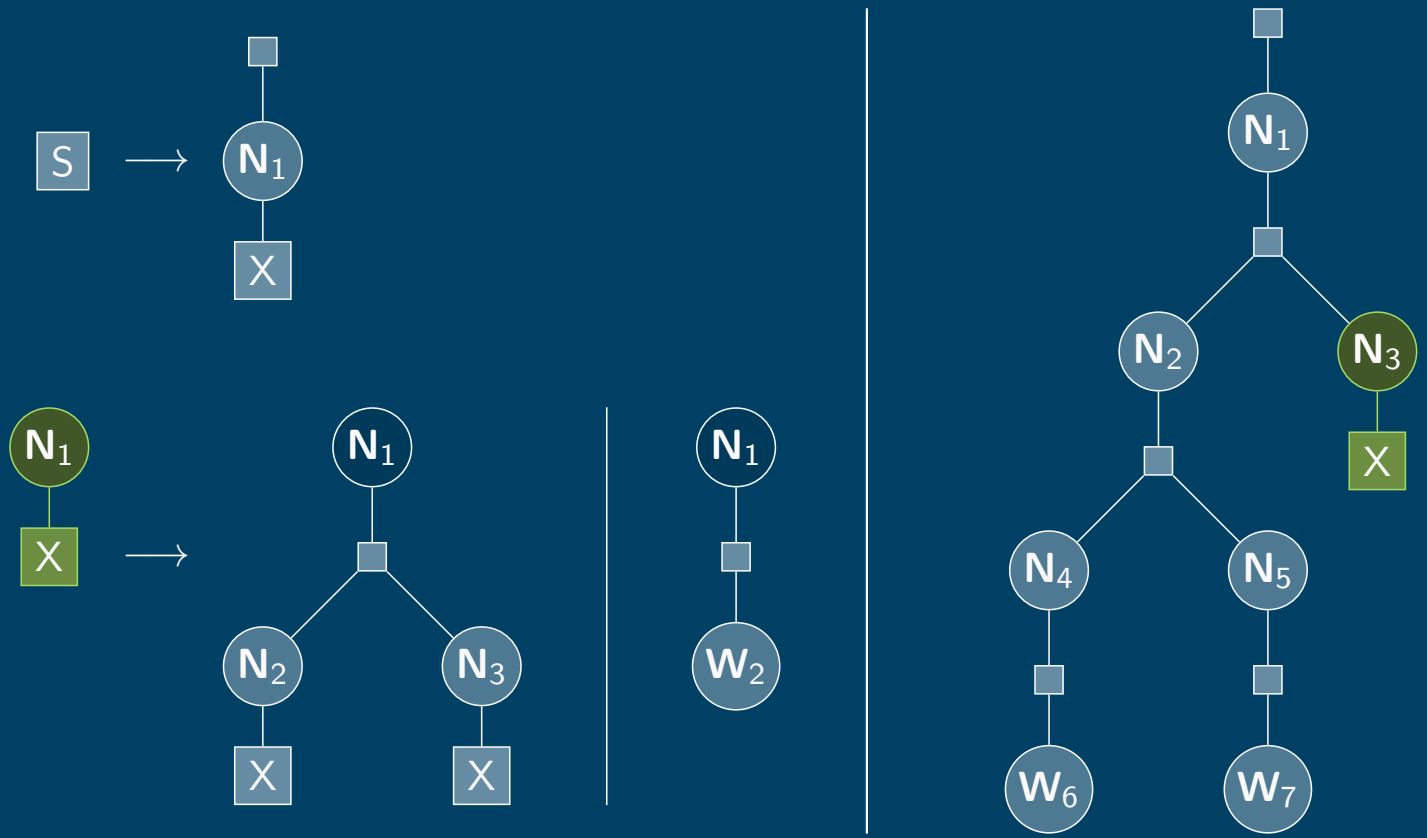

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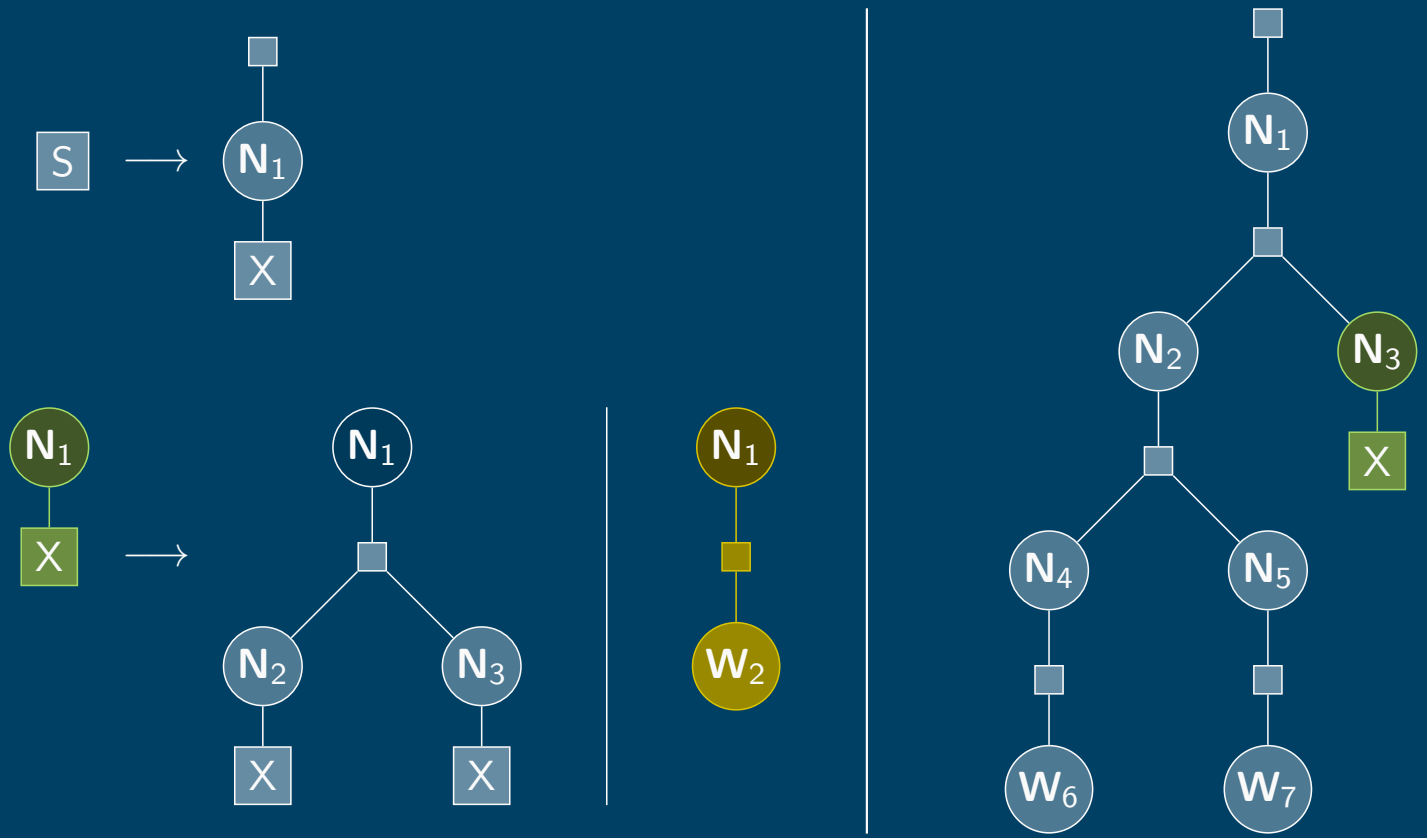

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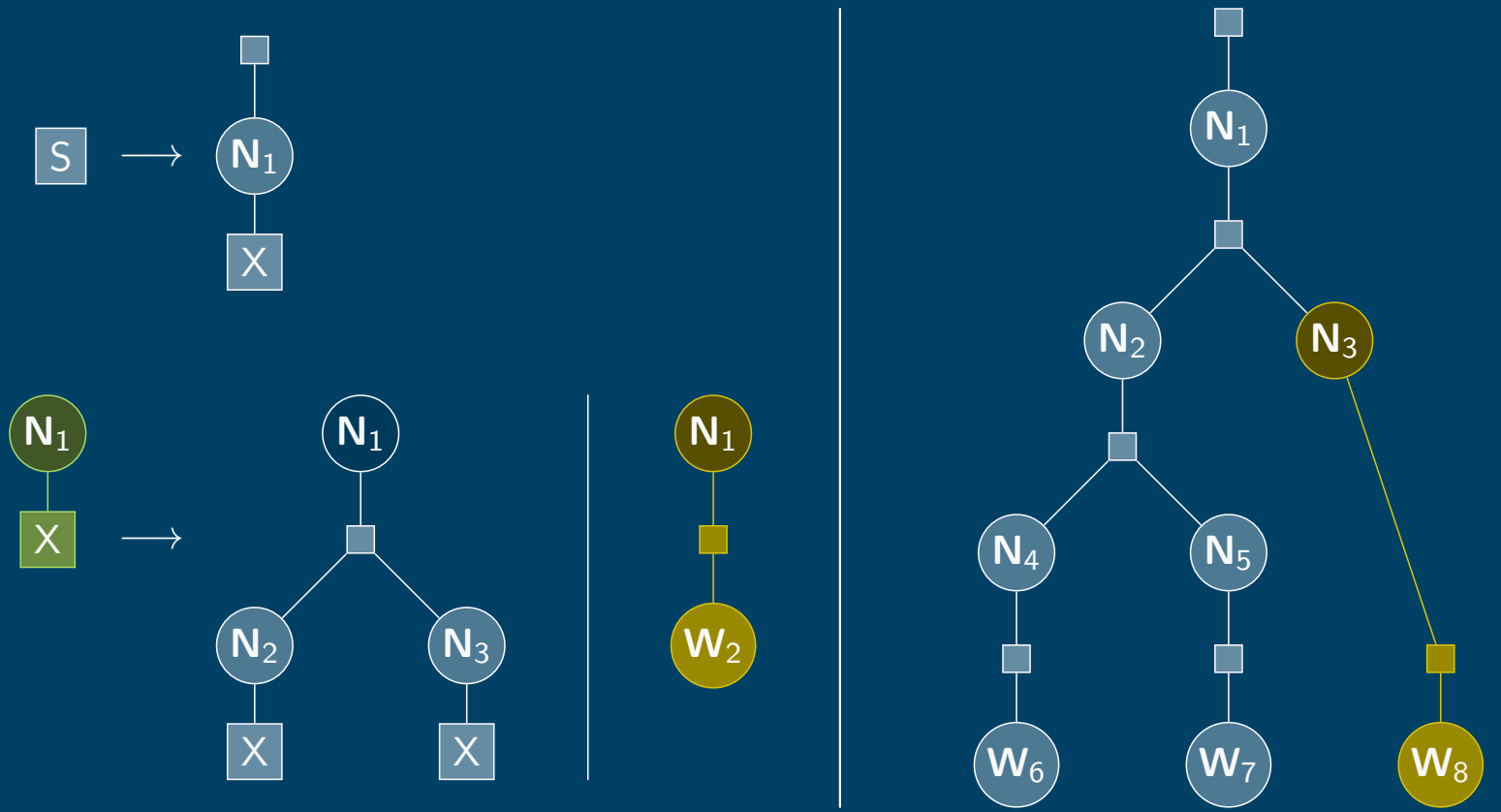

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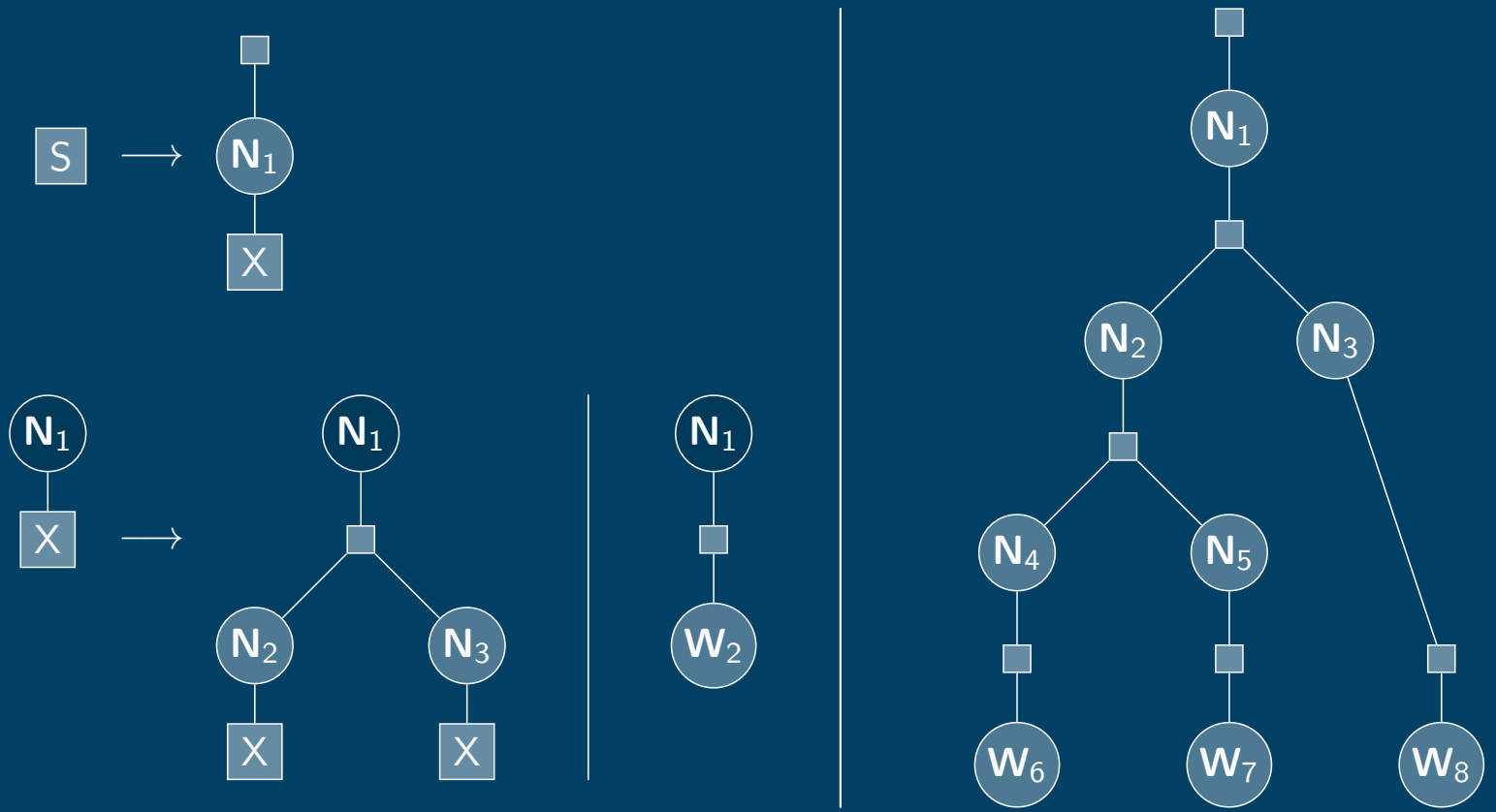


More FGG Ideas

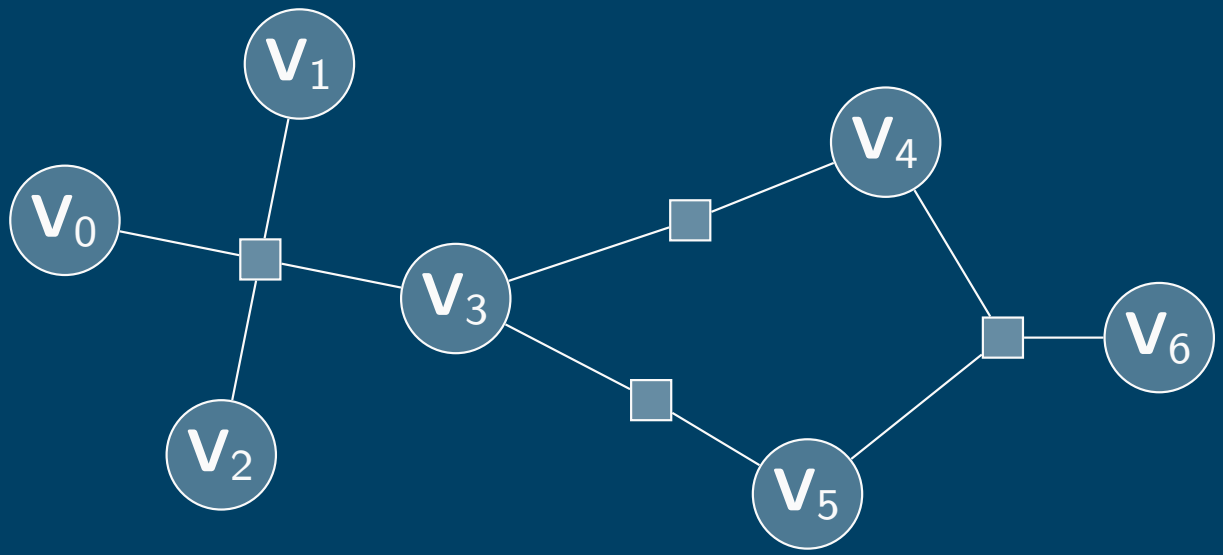
What else can you use FGGs for?

- Linear chains of nodes
- Anything tree-shaped (phylogeny trees, abstract syntax trees)
- More grammatical formalisms (TAG, LCFRS)
- Various types of DAGs (AMRs, control flow graphs, git commit histories?)
- RNA secondary structures

Sum-Product in a Factor Graph

Sum-Product in a Factor Graph

H:



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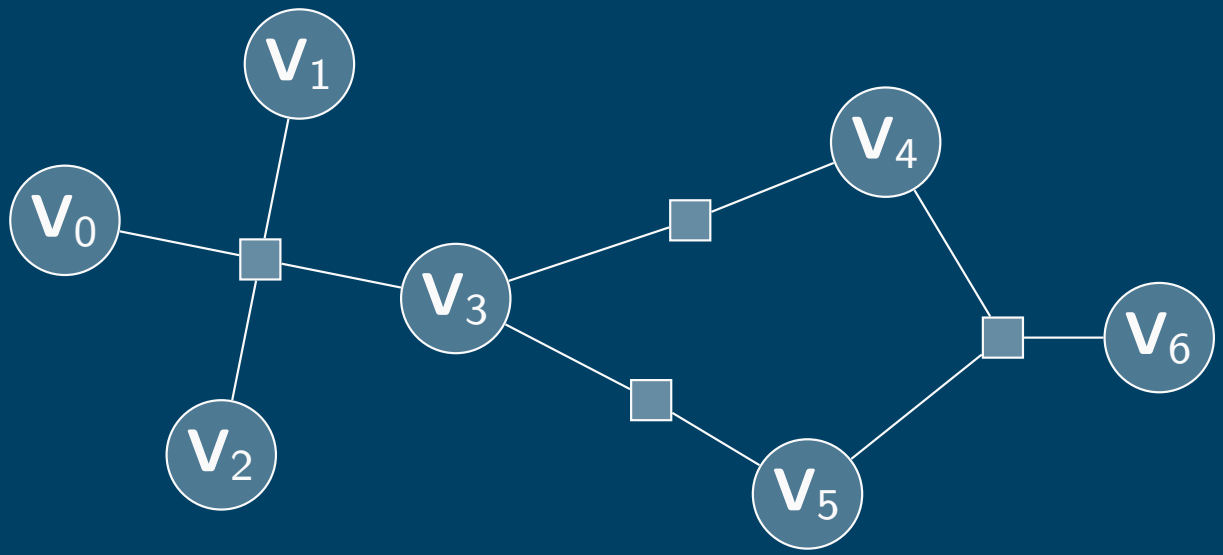

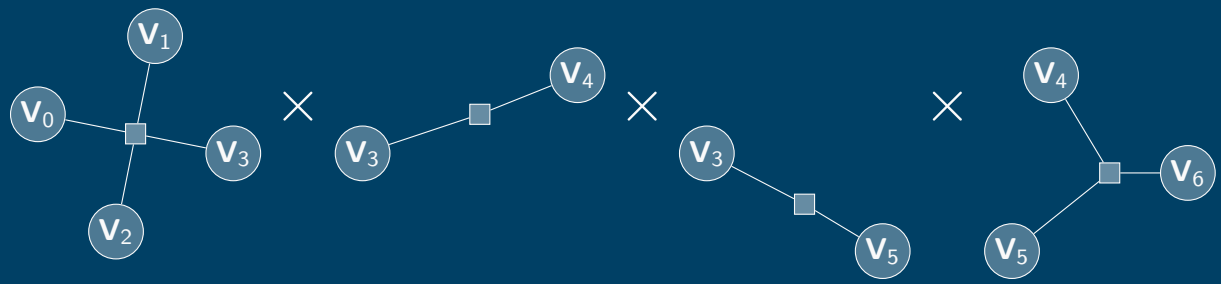

Sum-Product in a Factor Graph

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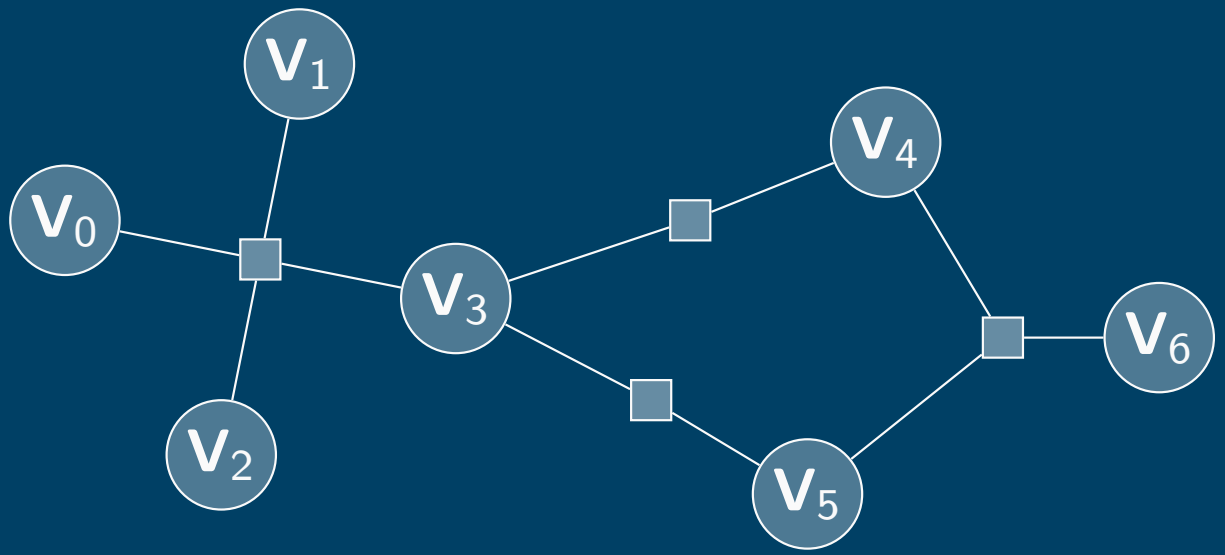
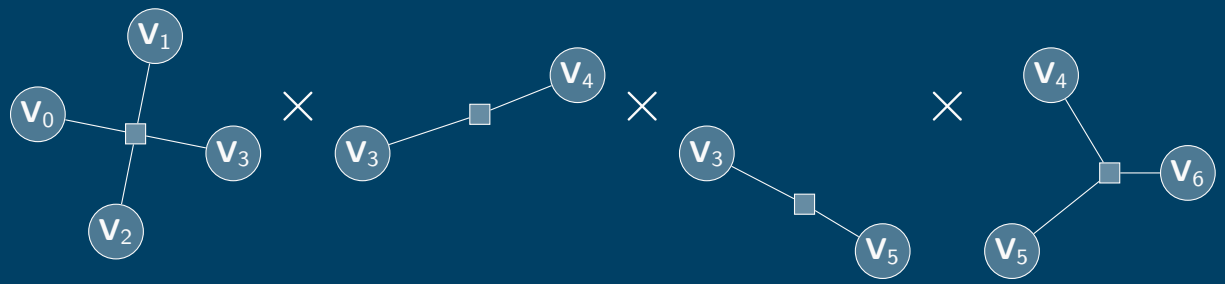


$$\frac{1}{Z}$$



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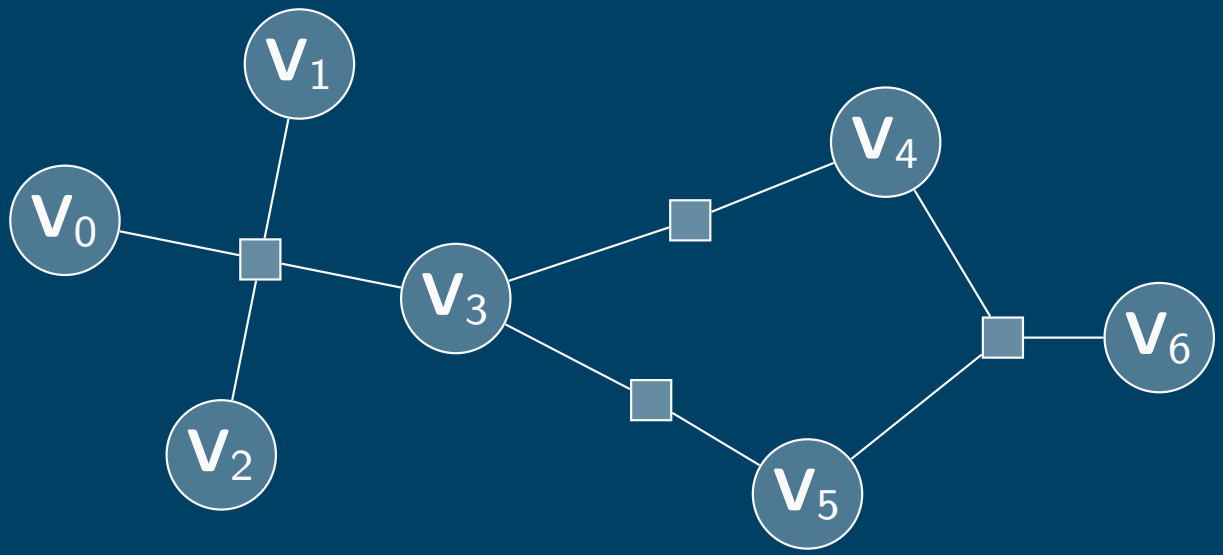
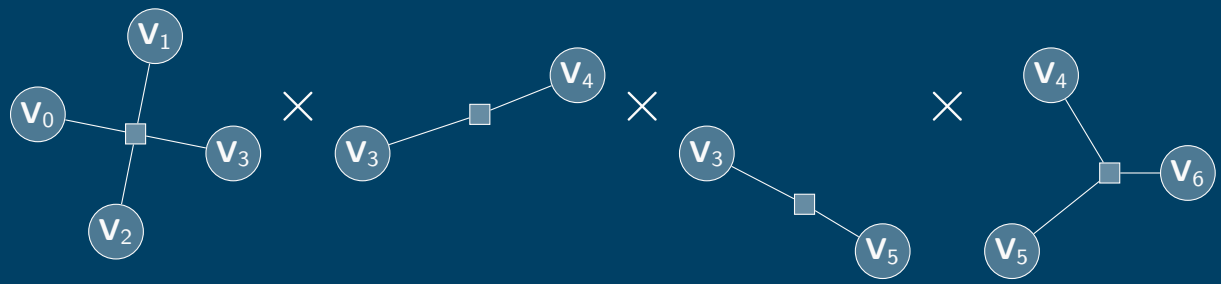


$Z(H) =$

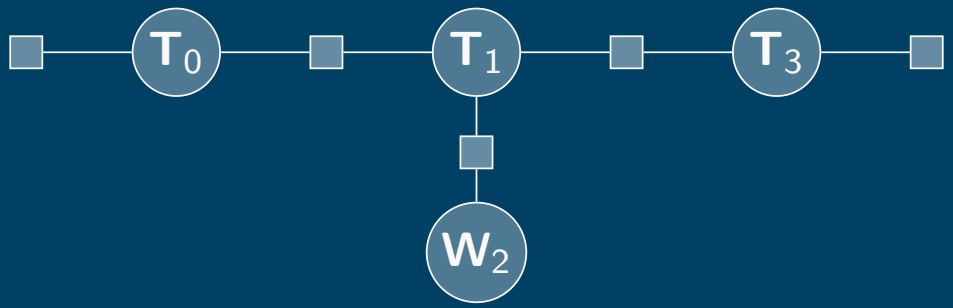
$$\sum_{\text{assignments to } V_0, V_1, \ldots, V_6}$$



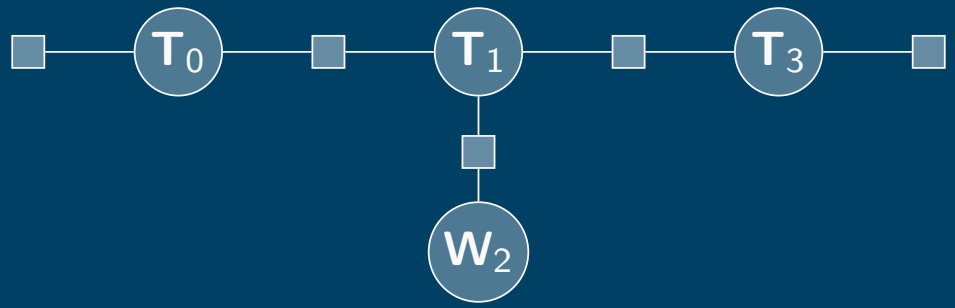
To compute sum-product of factor graph: sum over the weights of all assignments

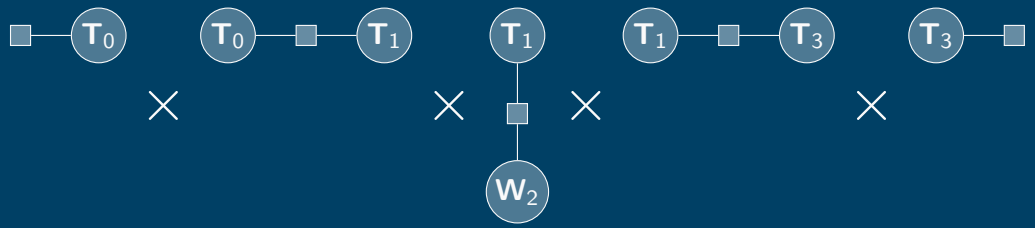
Sum-Product in a Factor Graph Grammar

Sum-Product in a Factor Graph Grammar



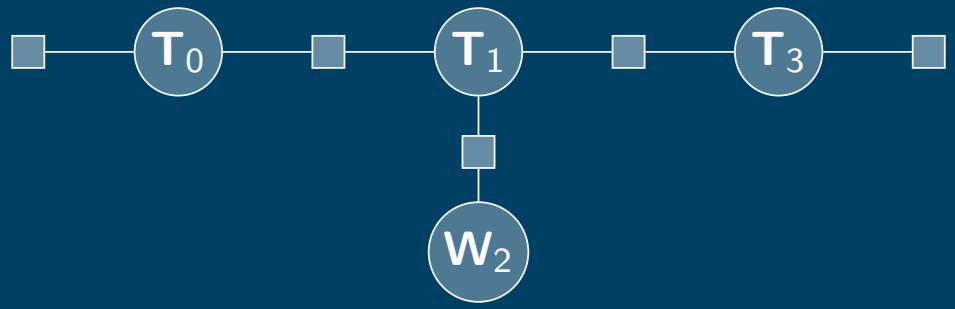
Sum-Product in a Factor Graph Grammar

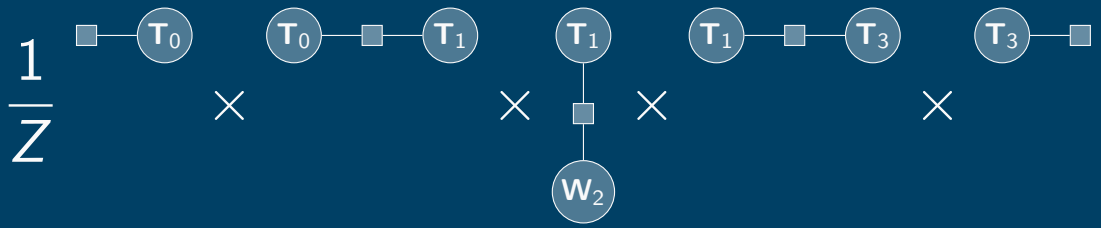




To compute weight of assignment: multiply factors together

Sum-Product in a Factor Graph Grammar

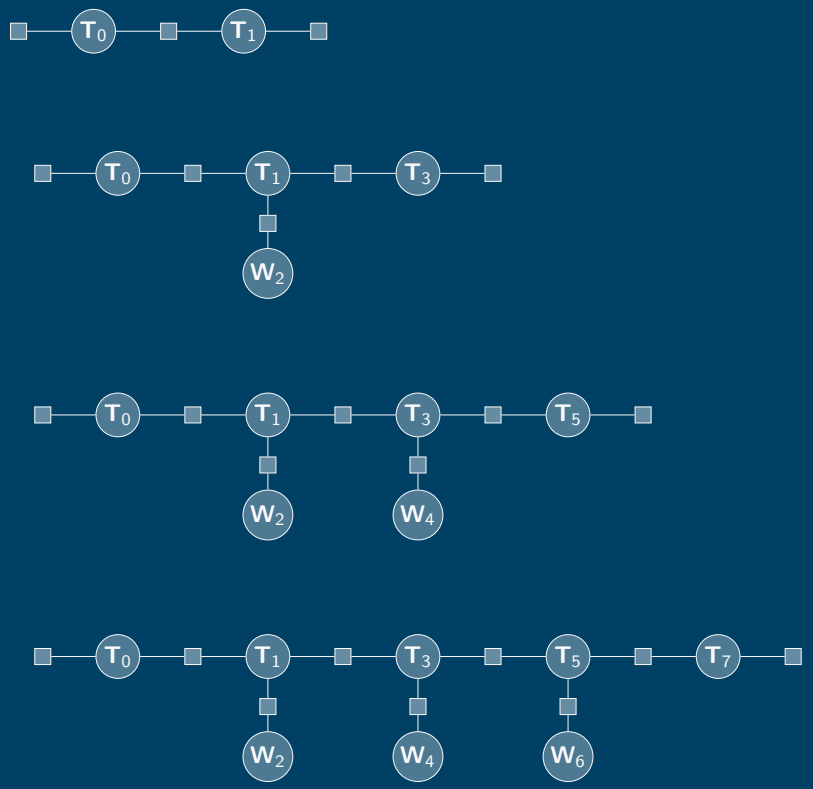




To convert weight to probability: divide by sum-product Z

Sum-Product in a Factor Graph Grammar

Sum-Product in a Factor Graph Grammar



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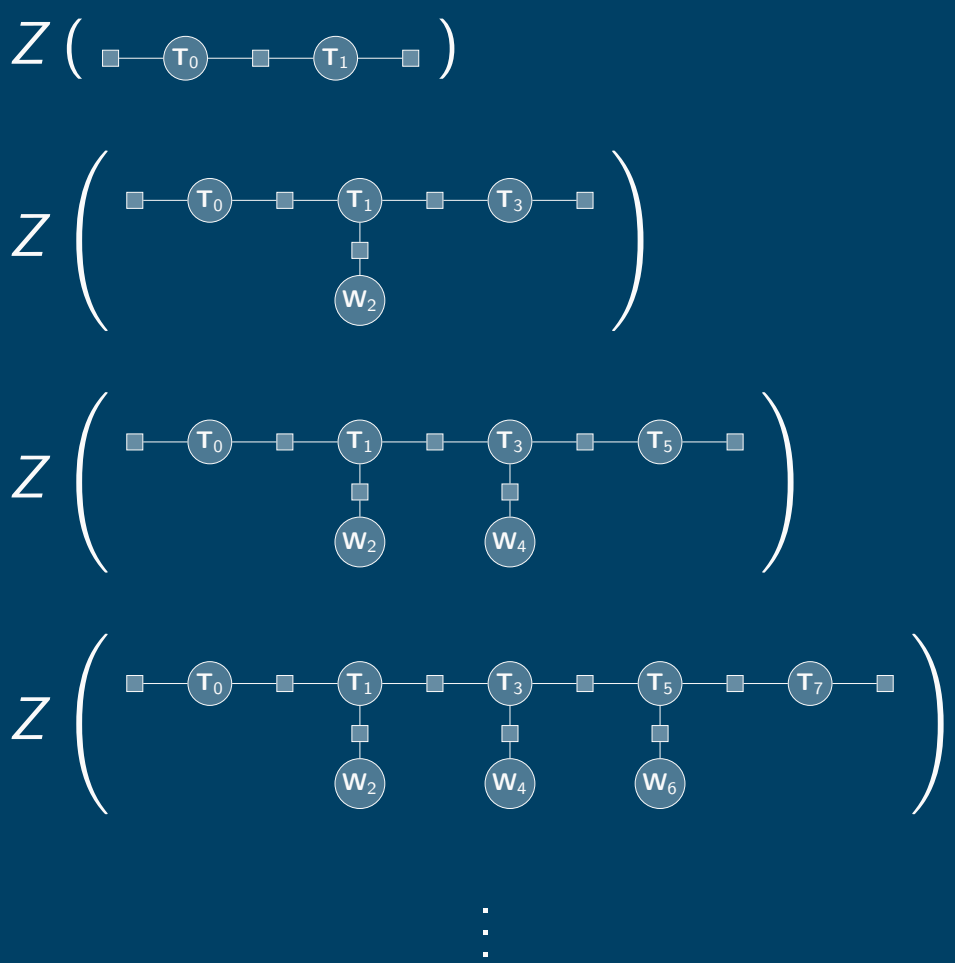
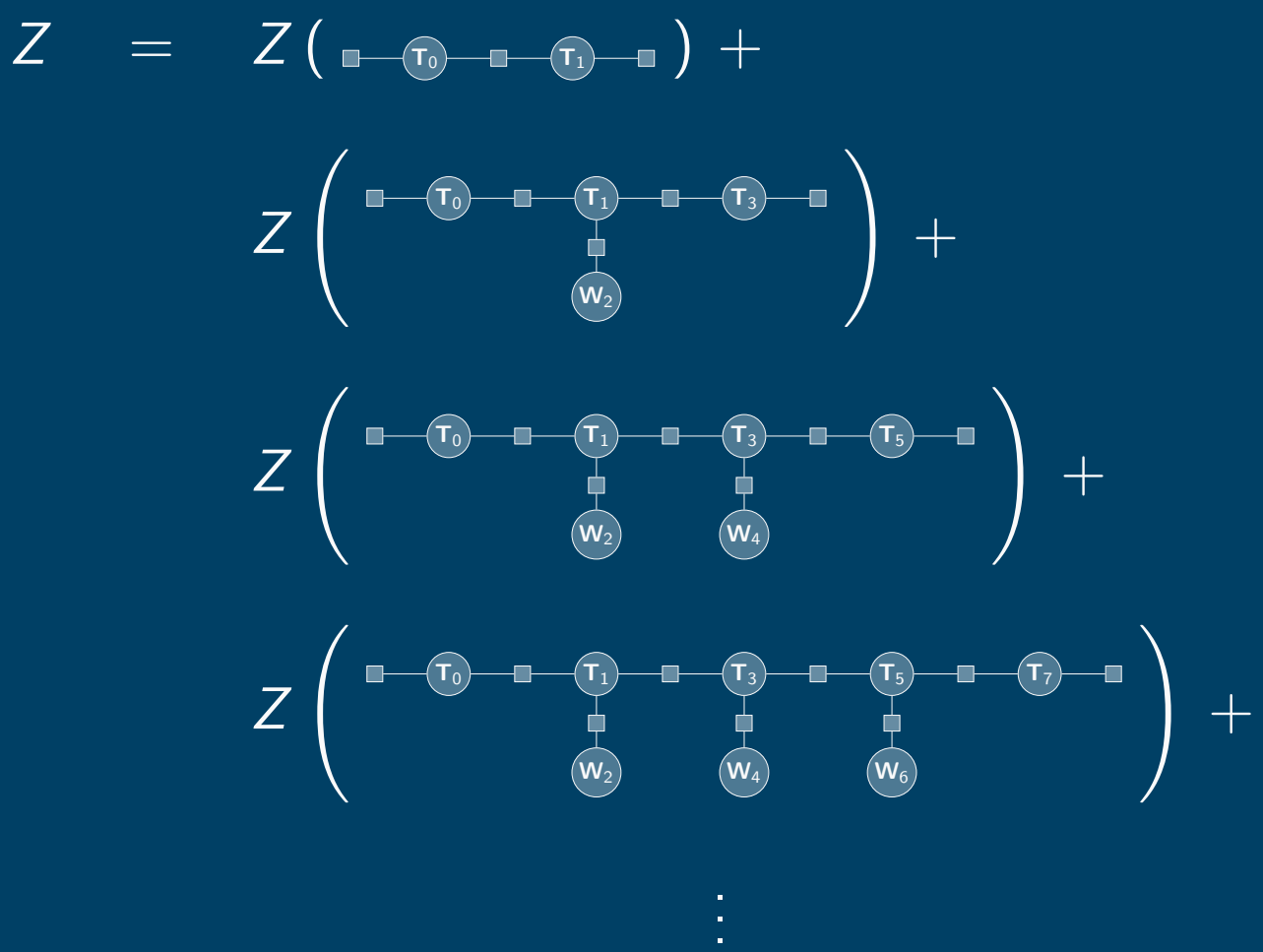


Sum-Product in a Factor Graph Grammar



To compute sum-product of factor graph grammar: sum over the sum-products of all derivations

Inference

Inference

3 cases:

- **Infinite graph language, finite variable domains:**
  use extension of variable elimination
- **Finite graph language, infinite variable domains:**
  convert to one big factor graph
- **Infinite graph language, infinite variable domains:**
  undecideable

Inference: Extending Variable Elimination

Can have infinite graphs, must have finite variable domains

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Write down a system of equations that lets us solve for Z:

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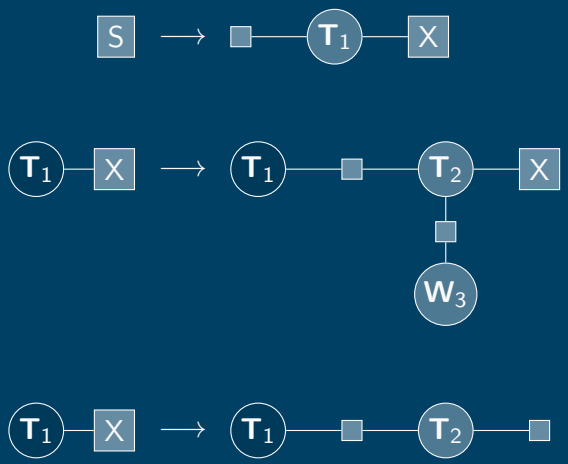
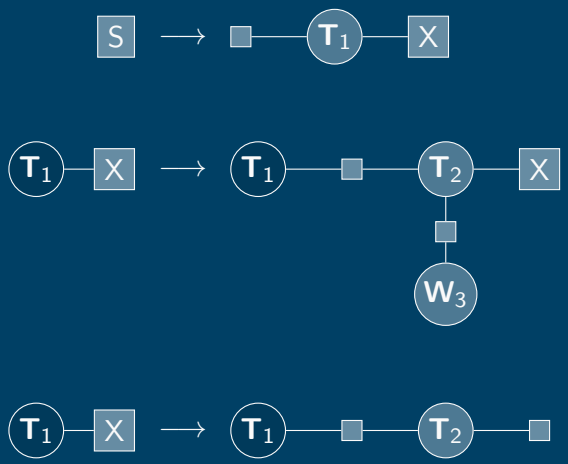


Inference: Extending Variable Elimination

Can have infinite graphs, must have finite variable domains

Write down a system of equations that lets us solve for Z:

- One eq. for each left-hand side + assignment to ext. nodes



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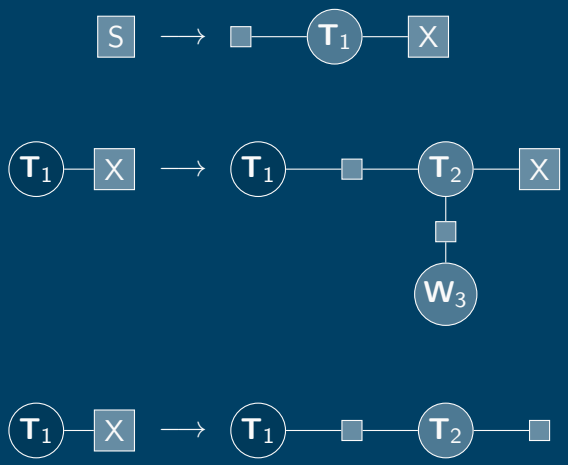

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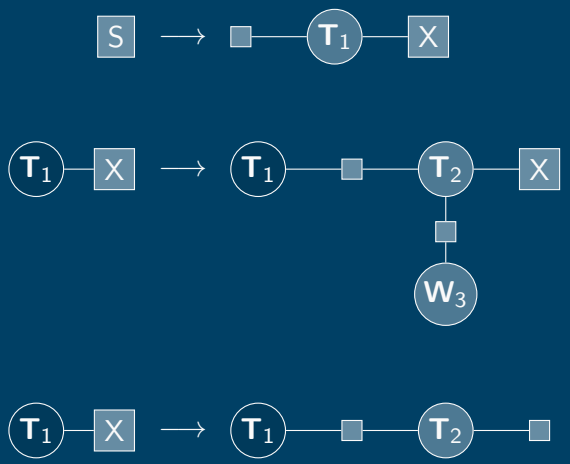


$$Z\left(\boxed{\text{S}}\right) = Z\left(\square\text{—}\boxed{\text{T}_1}\text{—}\boxed{\text{X}}\right)$$

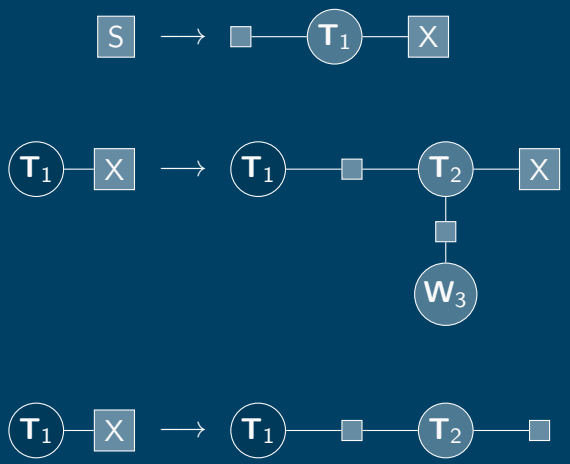
$$Z\left(\boxed{t_1}\text{—}\boxed{\text{X}}\right) = Z\left(\boxed{t_1}\text{—}\square\text{—}\boxed{\text{T}_2}\text{—}\boxed{\text{X}}\;;\;\boxed{\text{T}_2}\text{—}\square\text{—}\boxed{\text{W}_3}\right) + Z\left(\boxed{t_1}\text{—}\square\text{—}\boxed{\text{T}_2}\text{—}\square\right)$$

Inference: Extending Variable Elimination

Can have infinite graphs, must have finite variable domains

Write down a system of equations that lets us solve for Z:

- One eq. for each left-hand side + assignment to ext. nodes
- One eq. for each right-hand side + assignment to ext. nodes



$$Z\left(\square - \mathbf{T}_1 - \mathbf{X}\right) = \sum_{t_1 \in \mathbf{T}_1} \square - t_1 \times Z\left(t_1 - \mathbf{X}\right)$$

$$Z\left(t_1 - \square - \mathbf{T}_2 - \square\right) = \sum_{t_2 \in \mathbf{T}_2} t_1 - \square - t_2 \times t_2 - \square$$

Inference: Extending Variable Elimination

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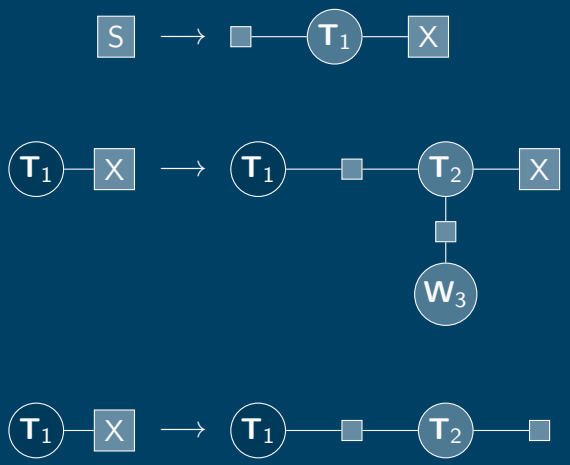
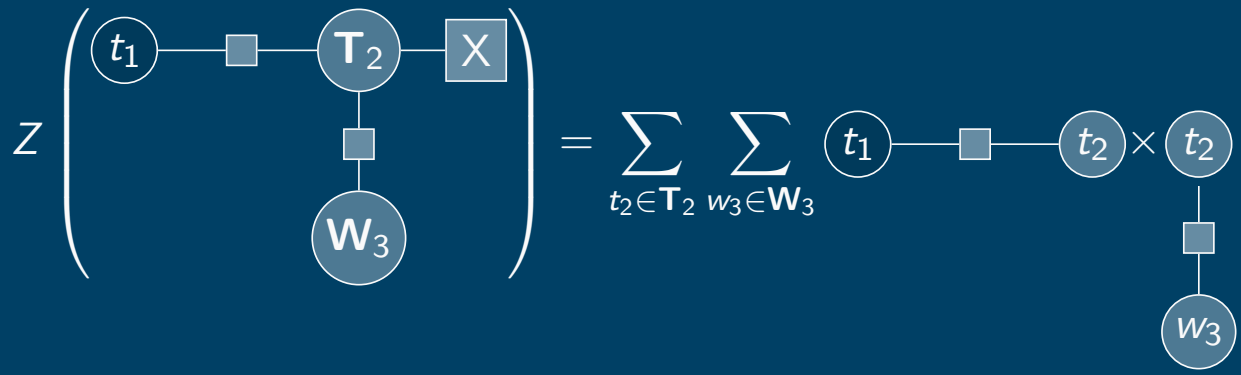
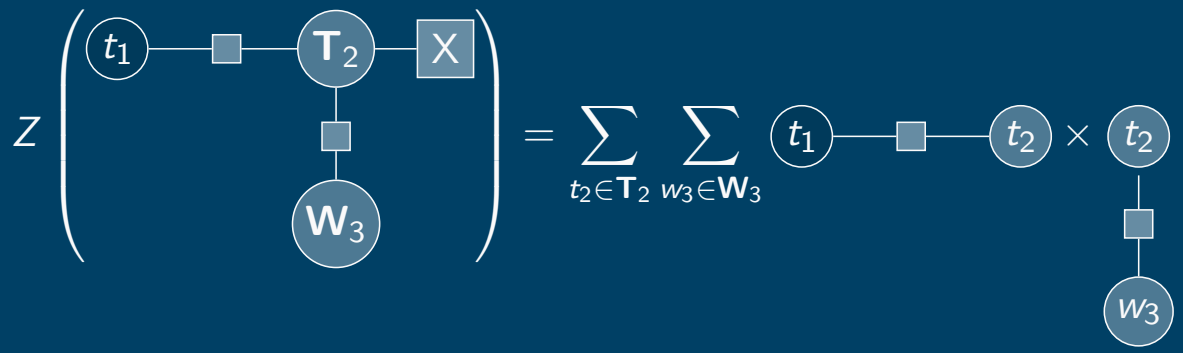




Computational Complexity



Number of equations: $O(|G|m^k)$

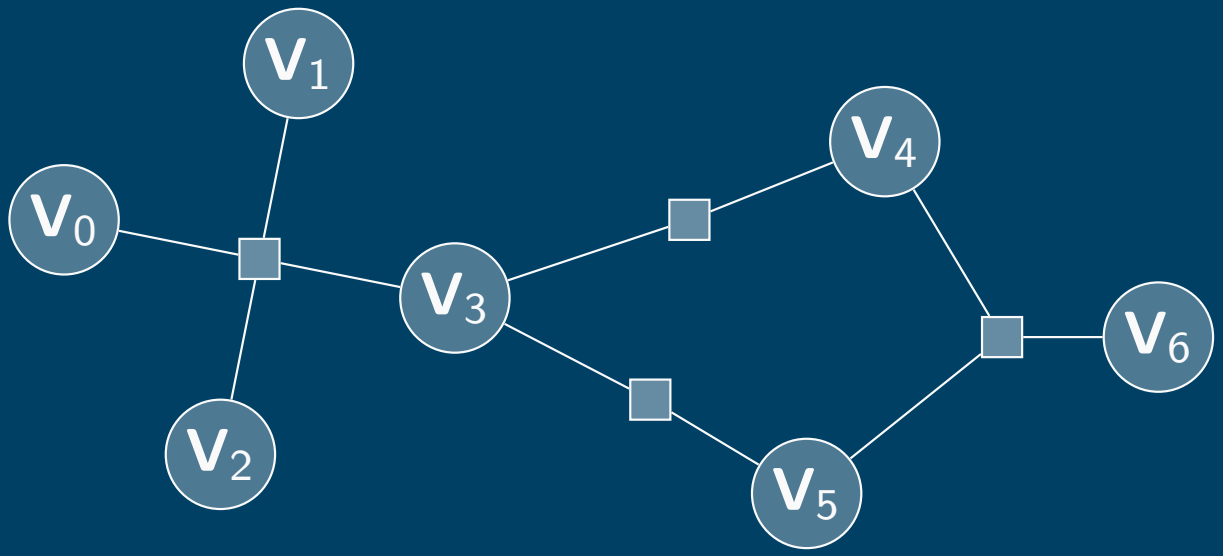
- $|G|$: number of rules
- m: max size of any variable domain
- k: max # of nodes in RHS

Cases:

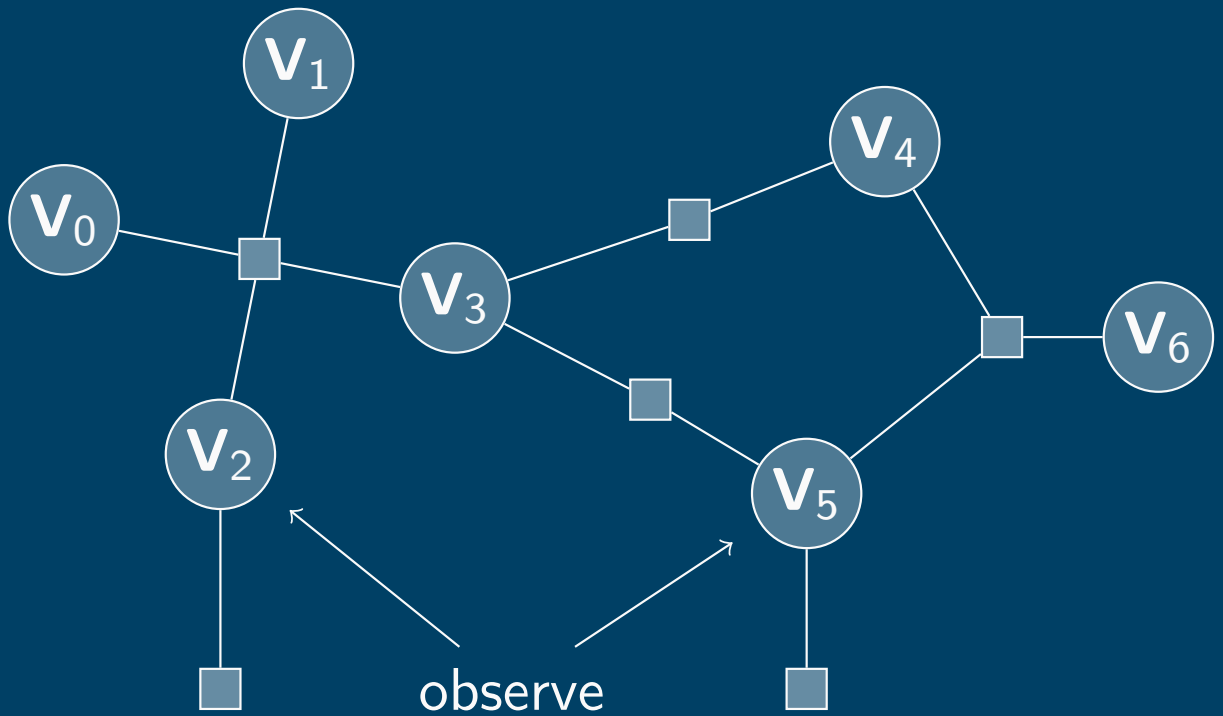
- **Non-recursive:** compute one at a time, $O(|G|m^k)$
- **Linear:** solve system of linear equations, $O(|G|^3 m^{3(k+1)})$
- **Otherwise:** solve iteratively

Querying a Factor Graph Grammar

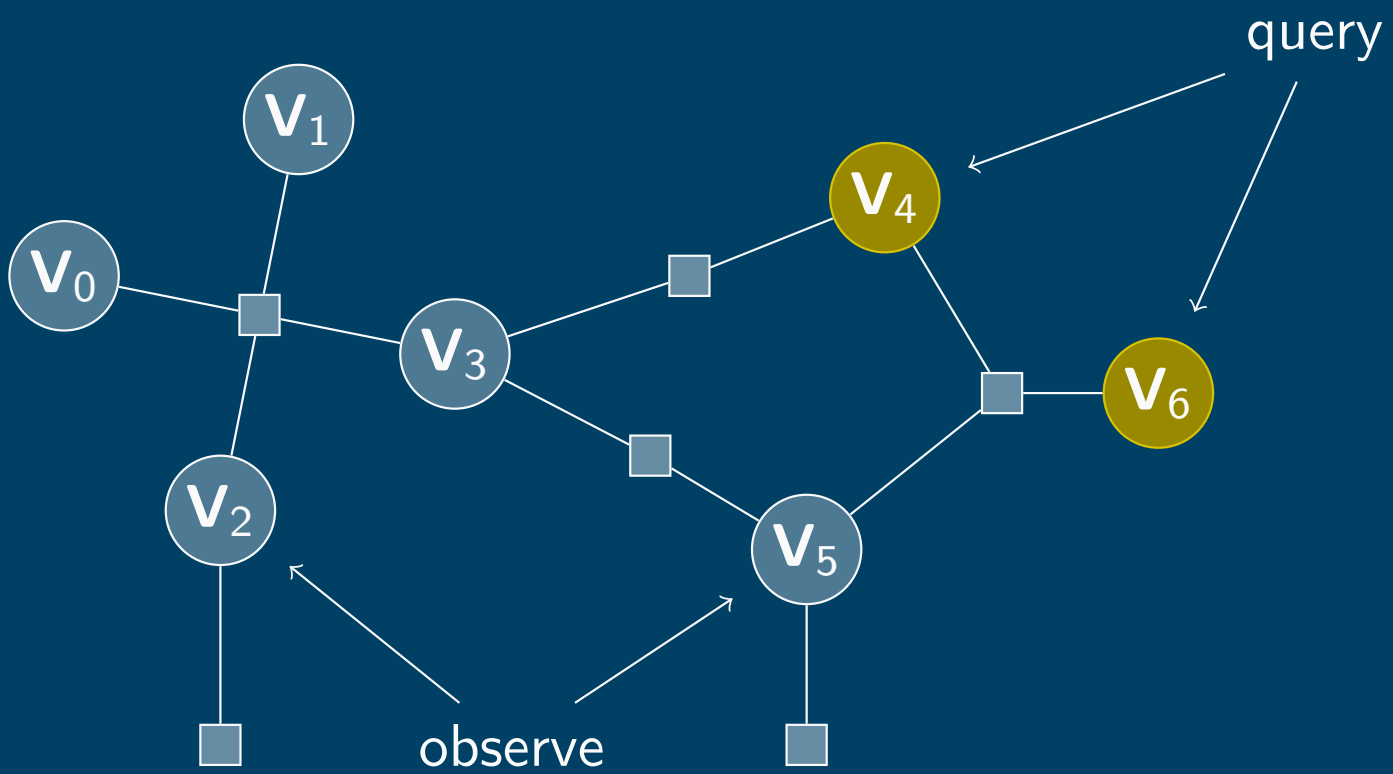
Queries



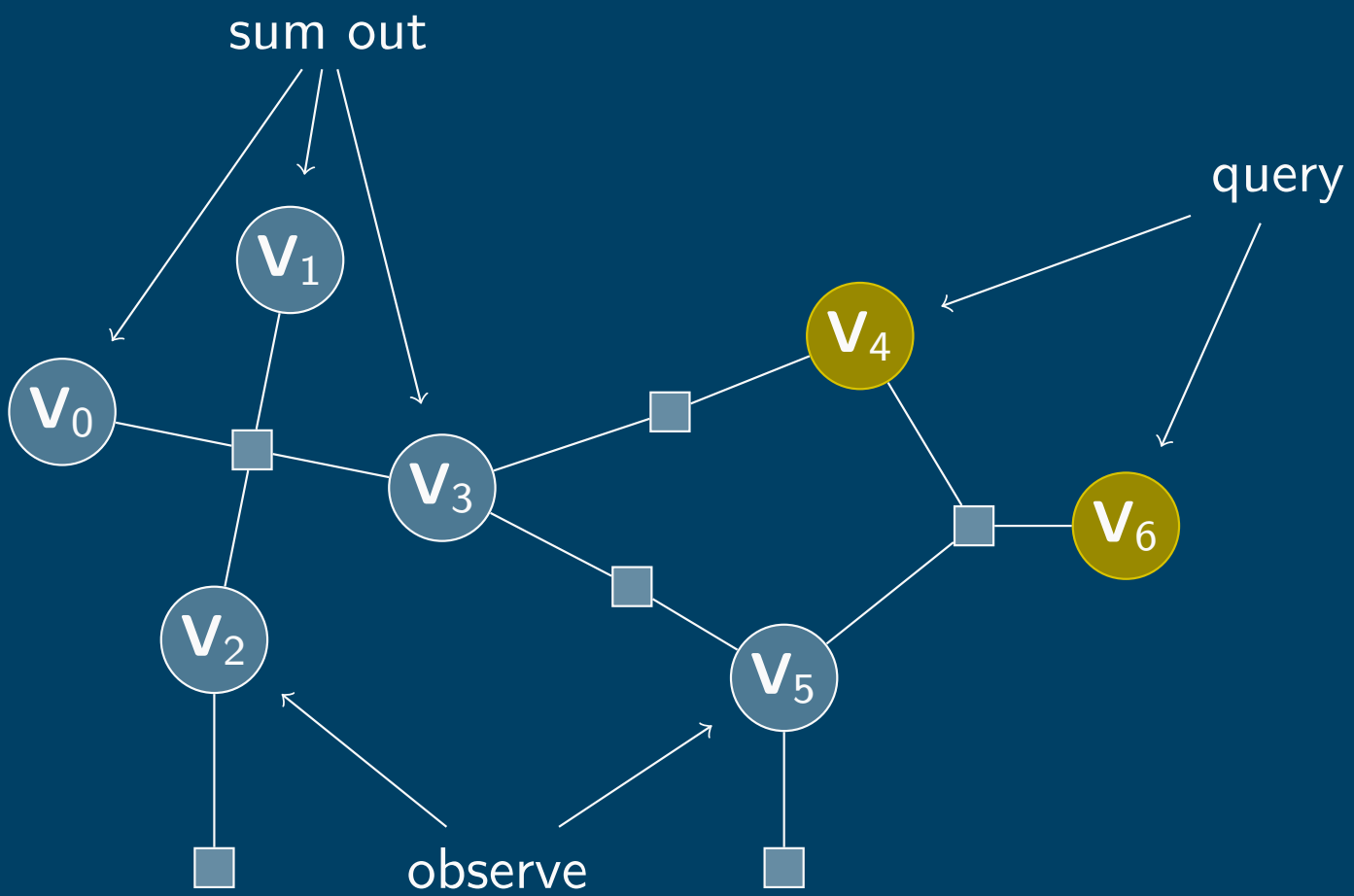
Queries



Queries

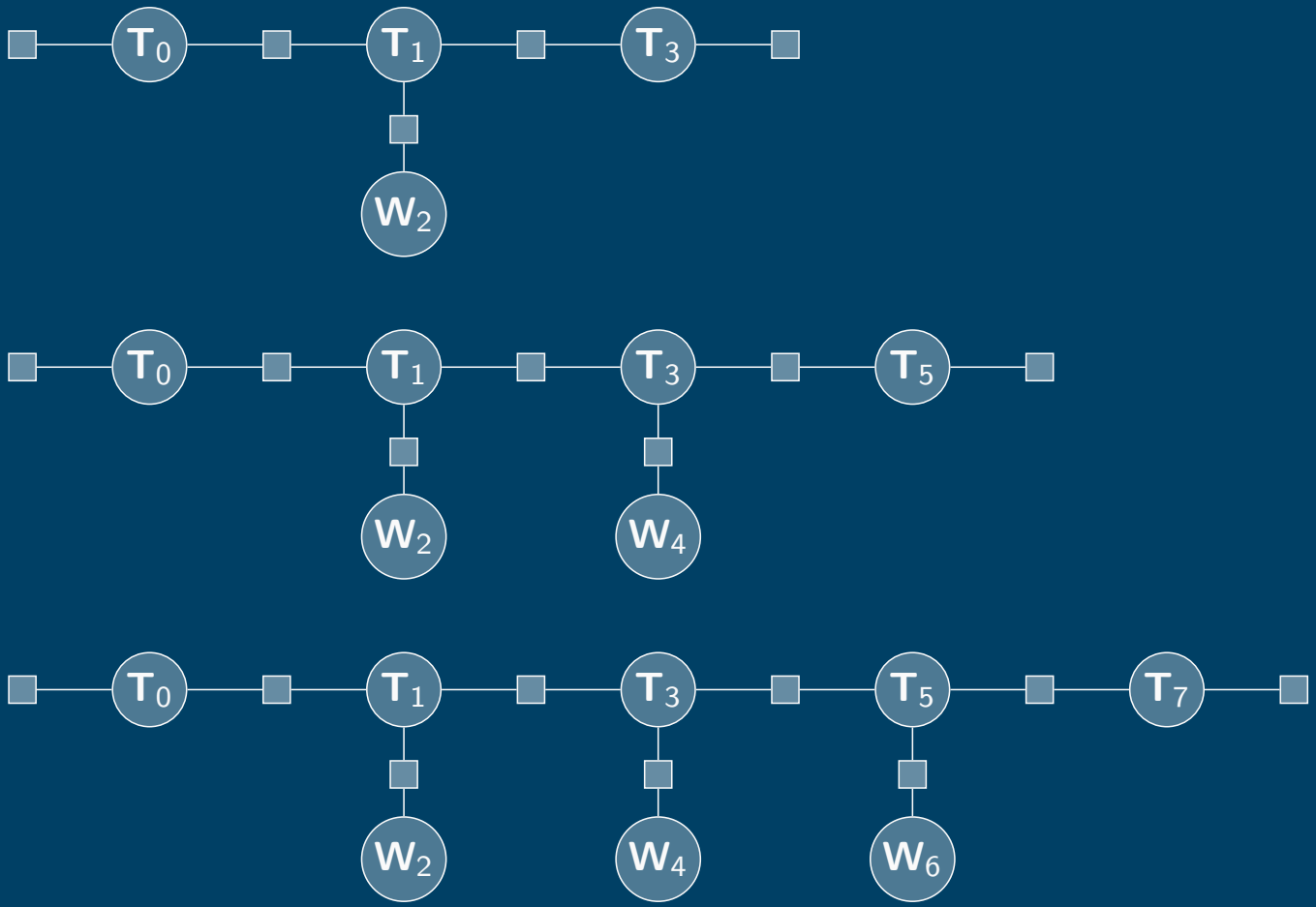


Queries



Queries

How to observe a value for the second-to-last tag?



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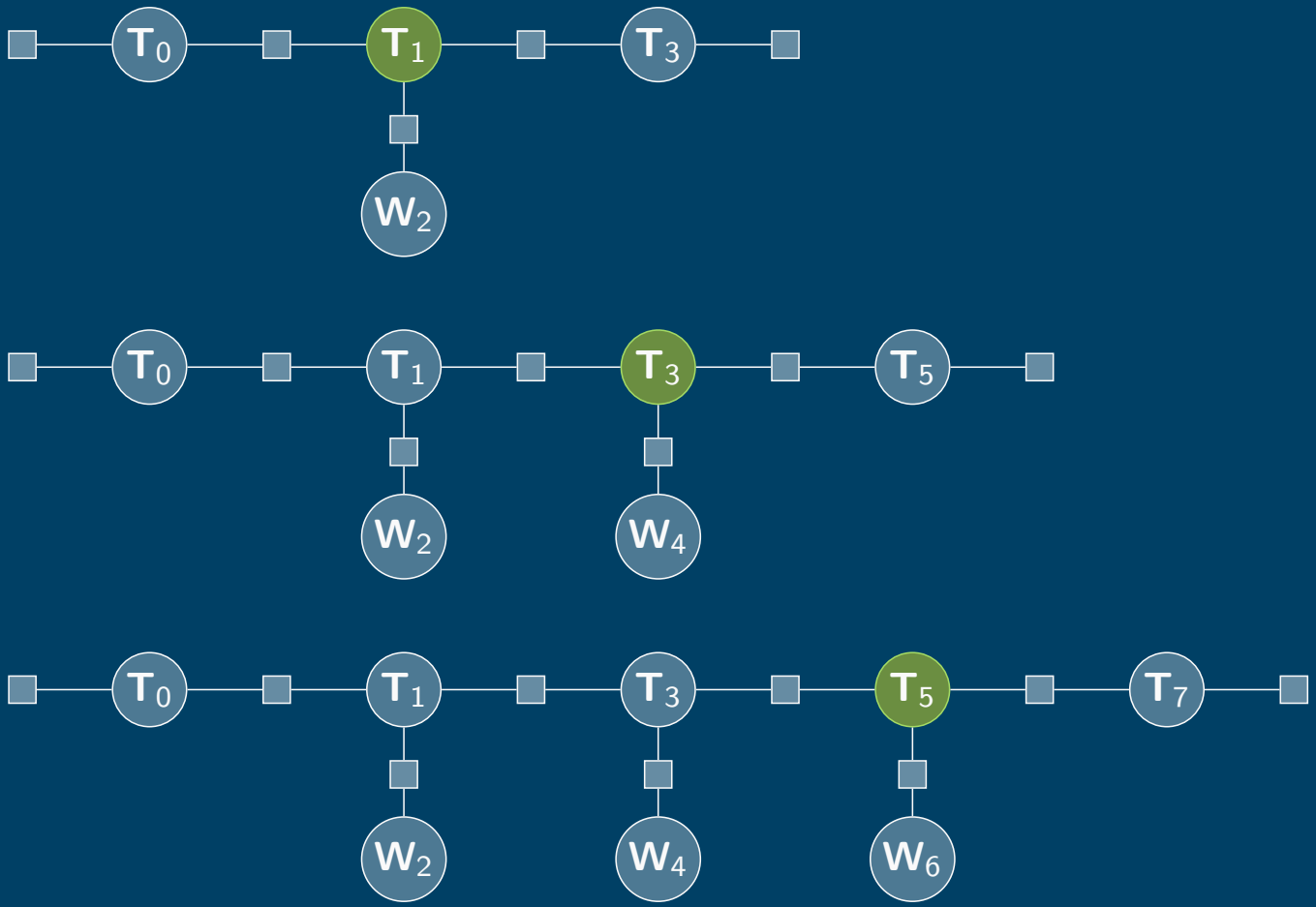
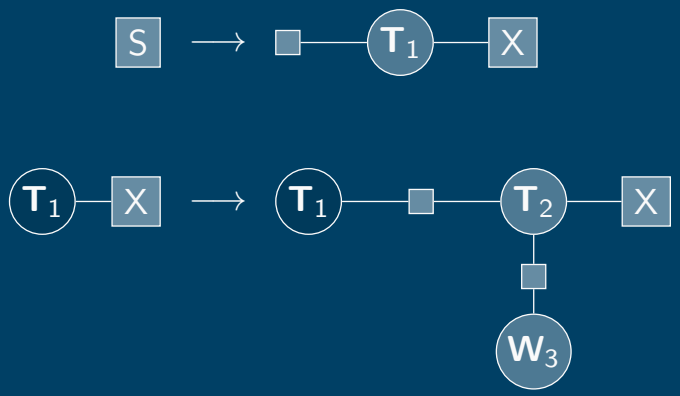


Queries

Instead of identifying variables in the derived graph,

identify variables in the grammar



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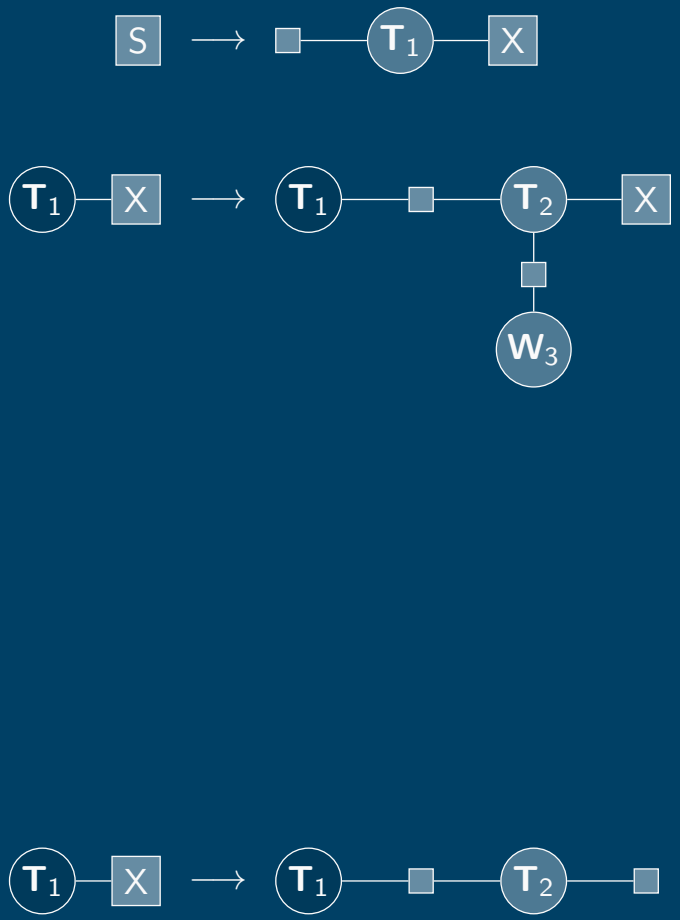

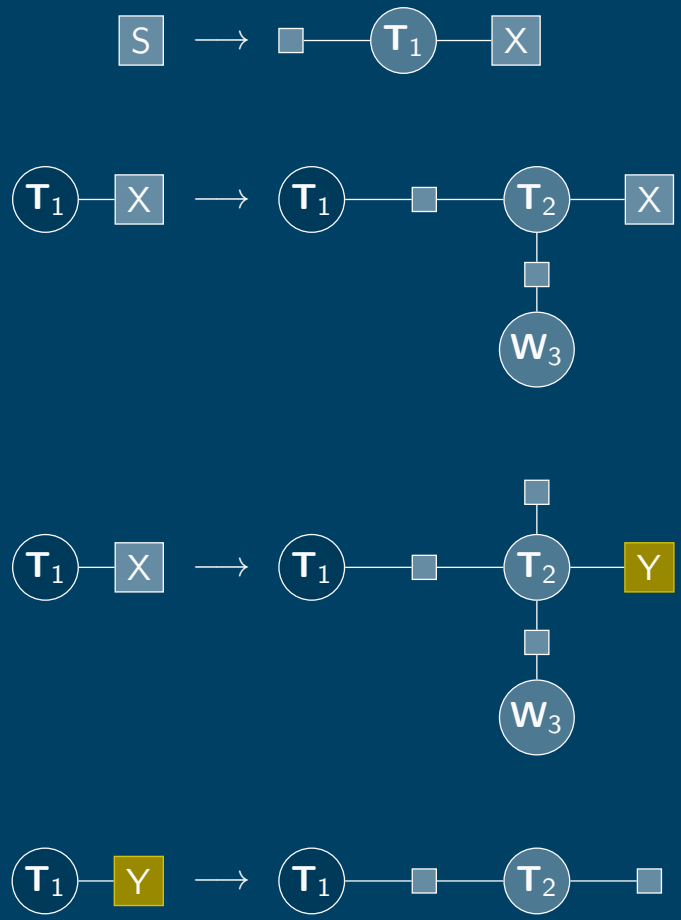

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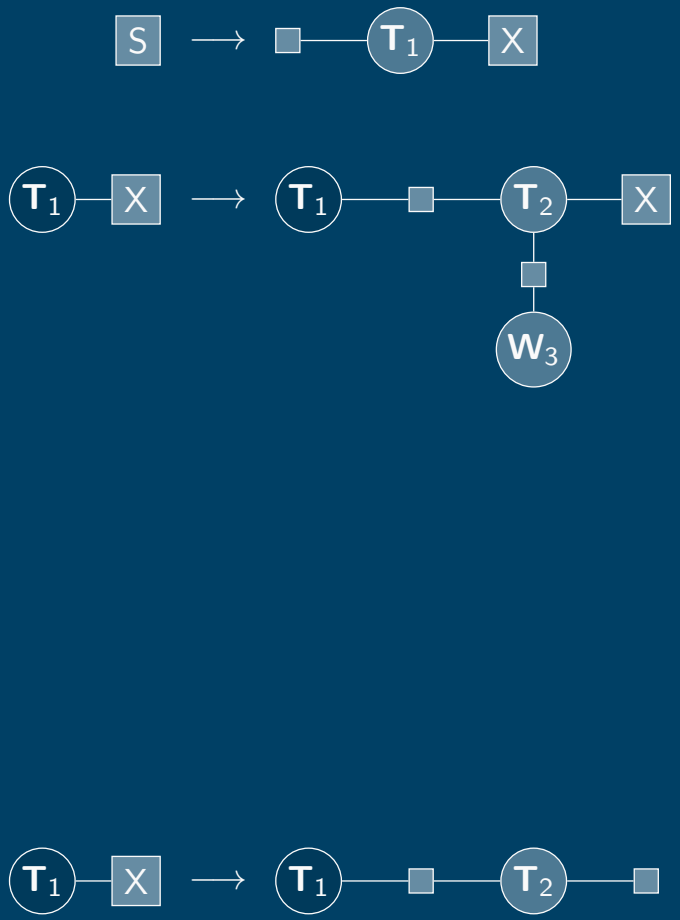

Conjunction

Conjunction lets you modularize grammar into two halves:

the original grammar and the query grammar

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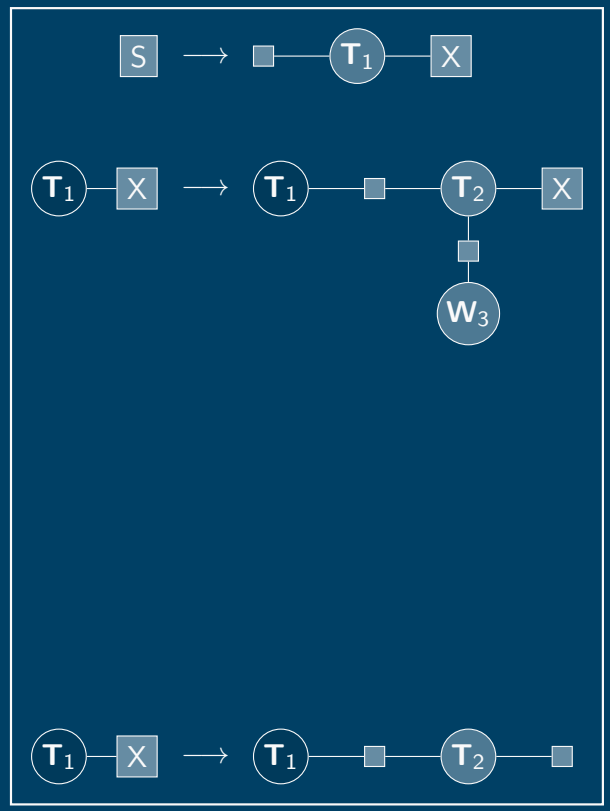

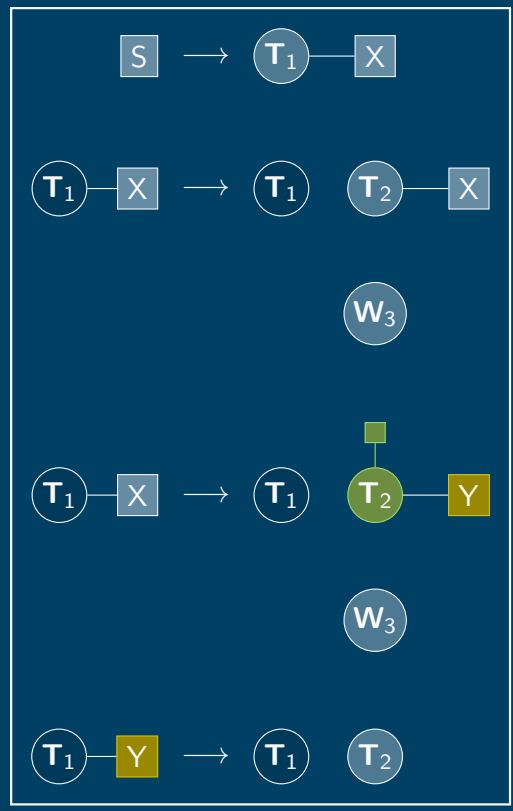

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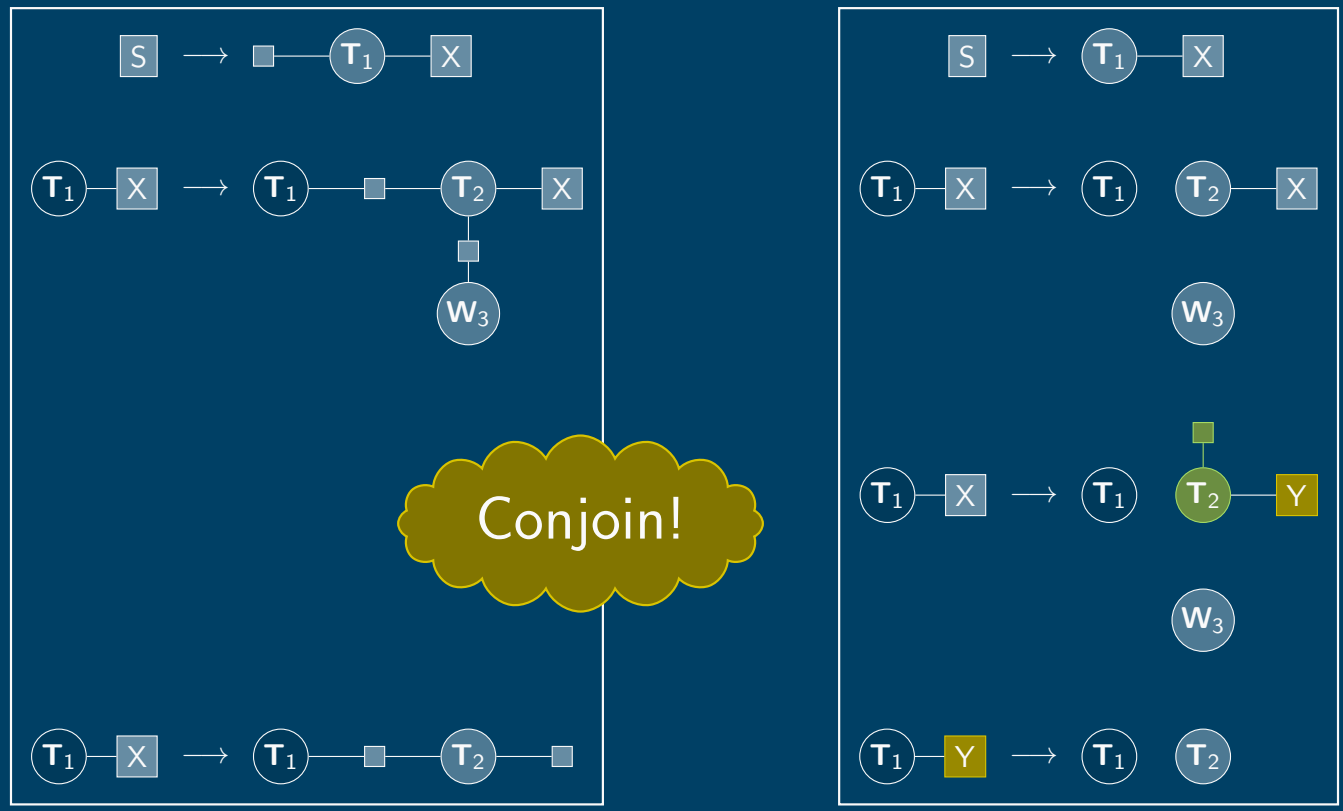

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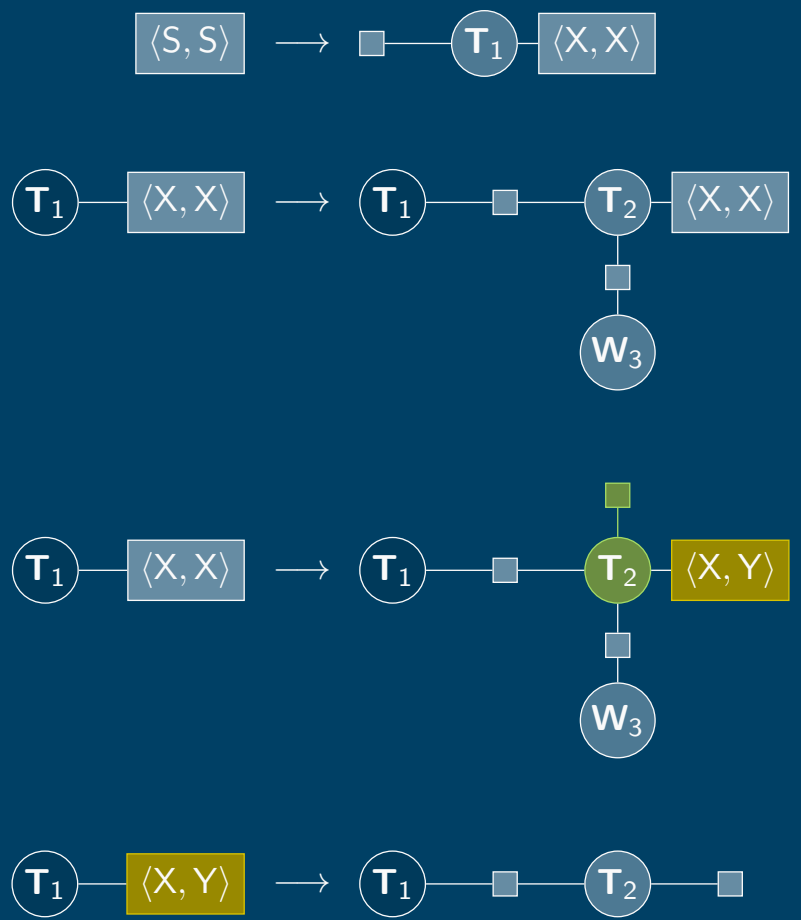

Related Work

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Lots of previous work generalizing PGMs.

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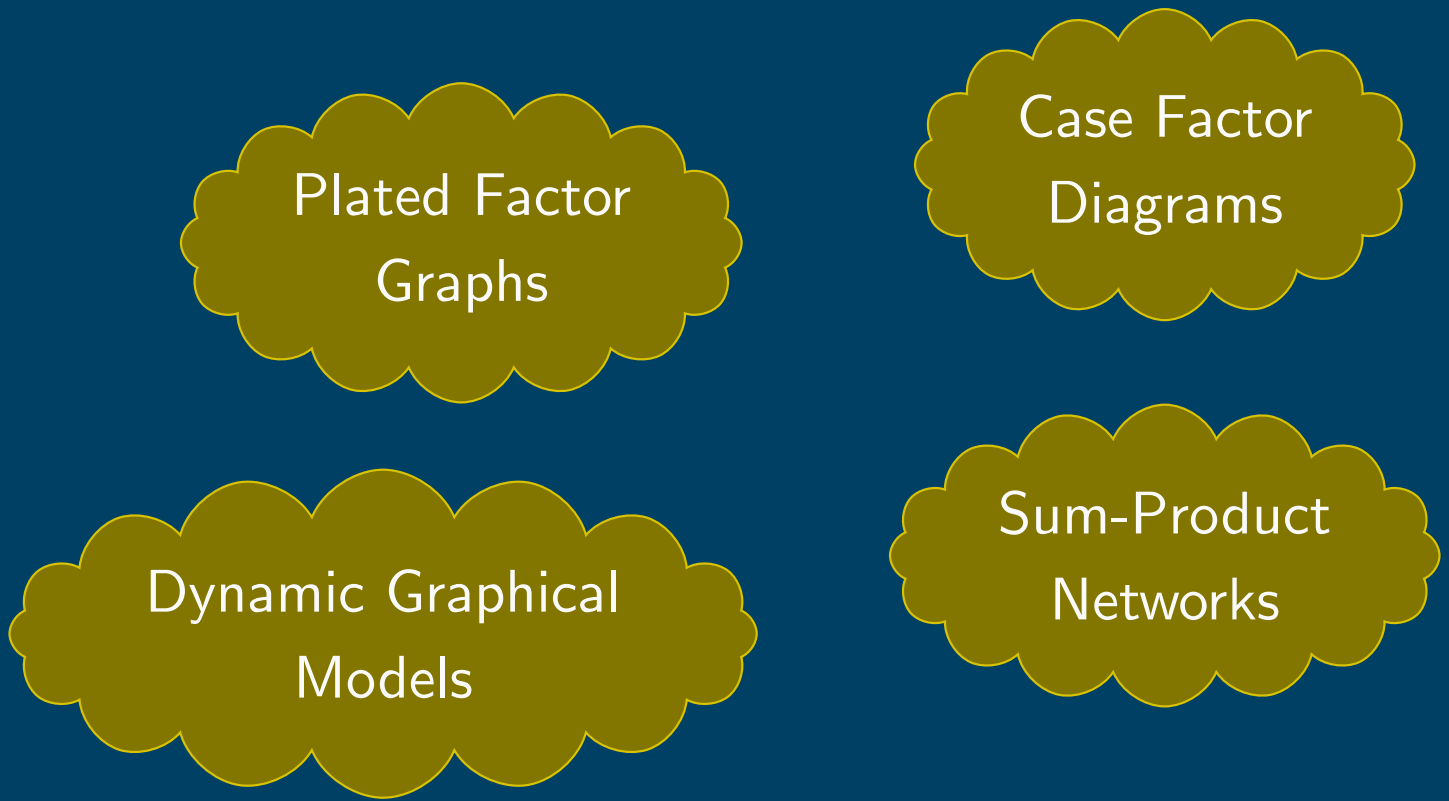
Tractable formalisms:



Related Work

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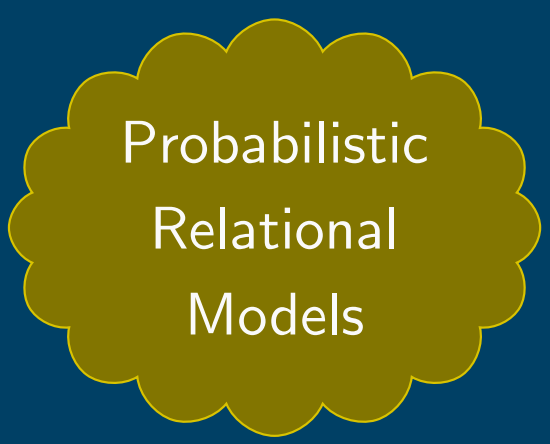
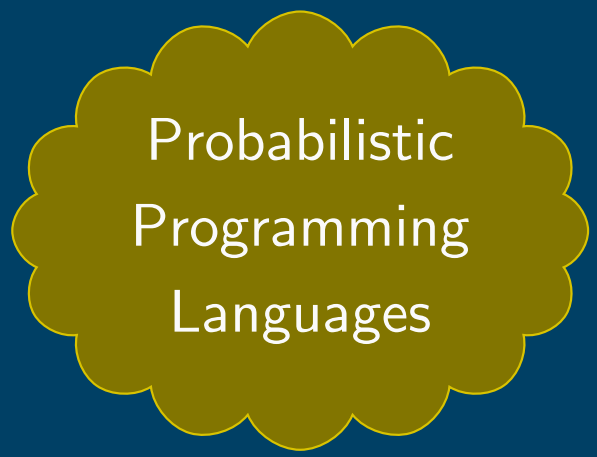
Expressive formalisms:





Related Work

Lots of previous work generalizing PGMs.

Factor graph grammars:

- General enough to subsume the tractable formalisms
- Simple enough to have tractable inference in many important cases

Ongoing and Future Work

Translating Recursive Probabilistic Programs to Factor Graph Grammars (PROBPROG 2020)

David Chiang
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Chung-chieh Shan
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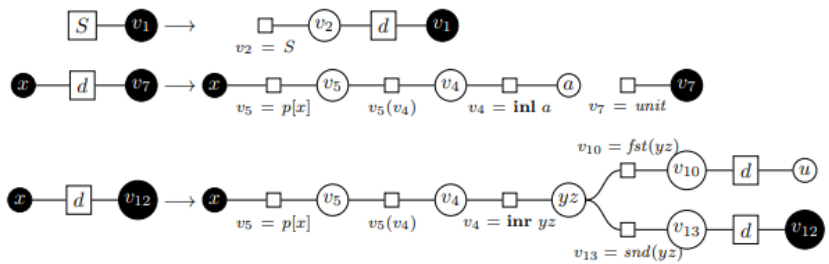
Chiang, David, and Chung-chieh Shan. "Translating Recursive Probabilistic Programs to Factor Graph Grammars." *arXiv preprint arXiv:2010.12071* (2020).

Translating Recursive Probabilistic Programs to Factor Graph Grammars (PROBPROG 2020)

```
# sample a tree from a PCFG
fun d(x) =
  case sample p[x] of
    inl a =>
      unit
  | inr yz =>
      let u = d(fst(yz)) in
      d(snd(yz));
d(S)
```

translates to



Future Work

- Implementation
- Approximate inference
- Better ways to query FGGs
- Automatic structure learning for FGG rules

Thank you!

References

Michel Bauderon and Bruno Courcelle. 1987. Graph expressions and graph rewriting. *Mathematical Systems Theory*, 20:83–127.

Annegret Habel and Hans-Jörg Kreowski. 1987. May we introduce to you: Hyperedge replacement. In *Proc. Third International Workshop on Graph Grammars and Their Application to Computer Science*, pages 15–26.