Graph search for inference

Neuro-symbolic modeling

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The problem

Suppose we have a problem of assigning labels to n different variables

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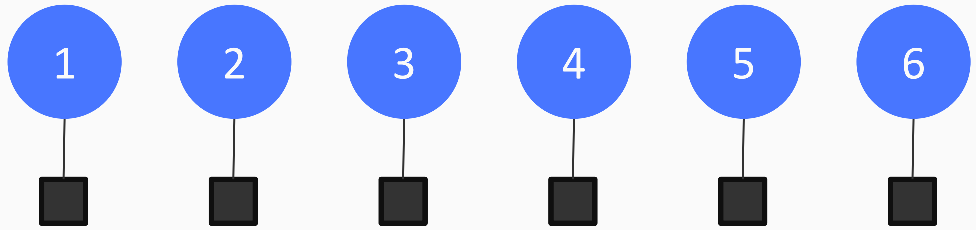
- Each label assignment has a score



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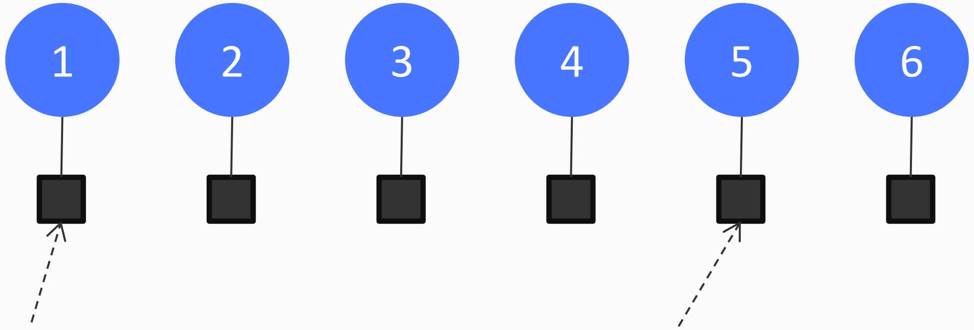

Scores of label assignments of variable 1

Scores of label assignments of variable 5

Each of these scores could be generated by a neural network

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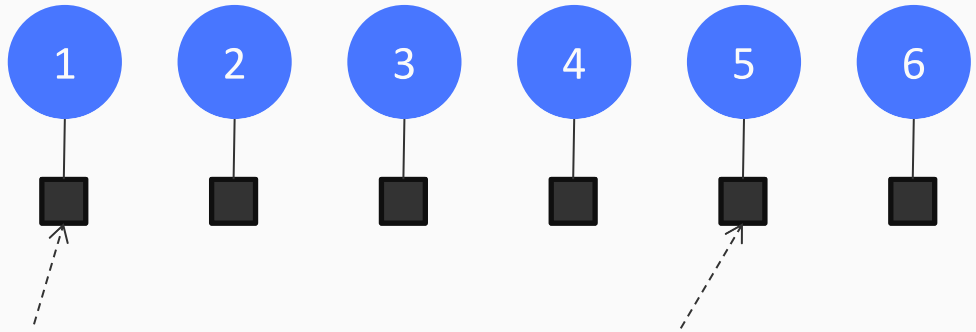
  - could be hard constraints

    e.g. `if label1=A then label2=B`



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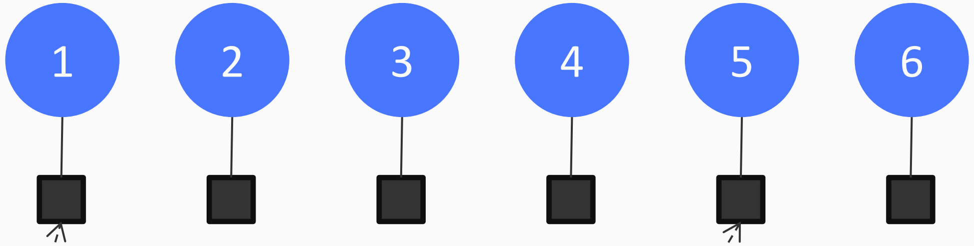
    e.g. score(label1=A, label2=B) = -40



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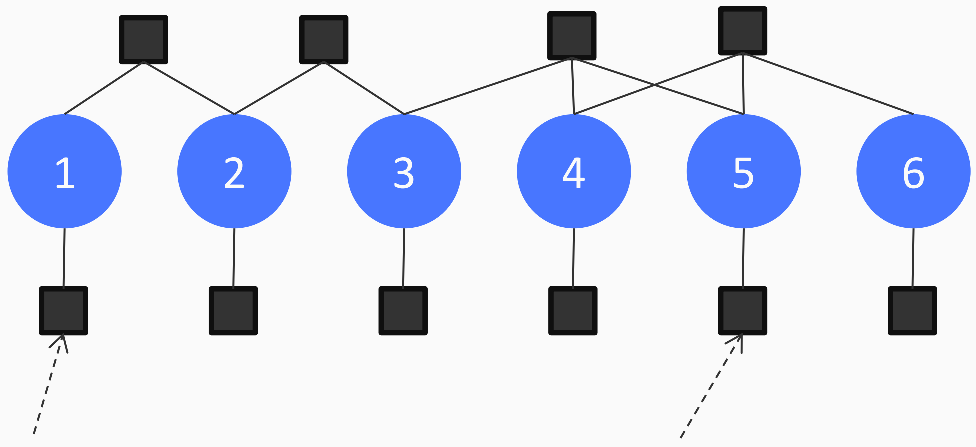

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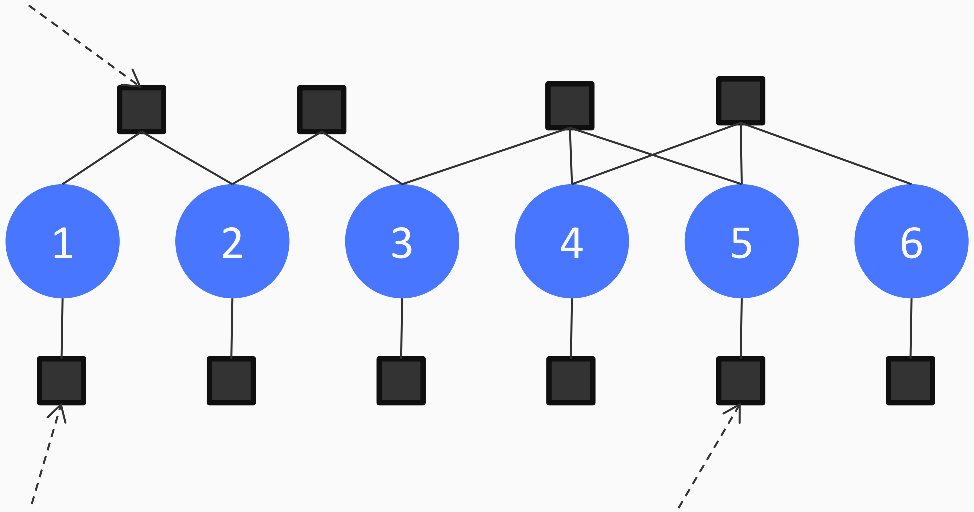

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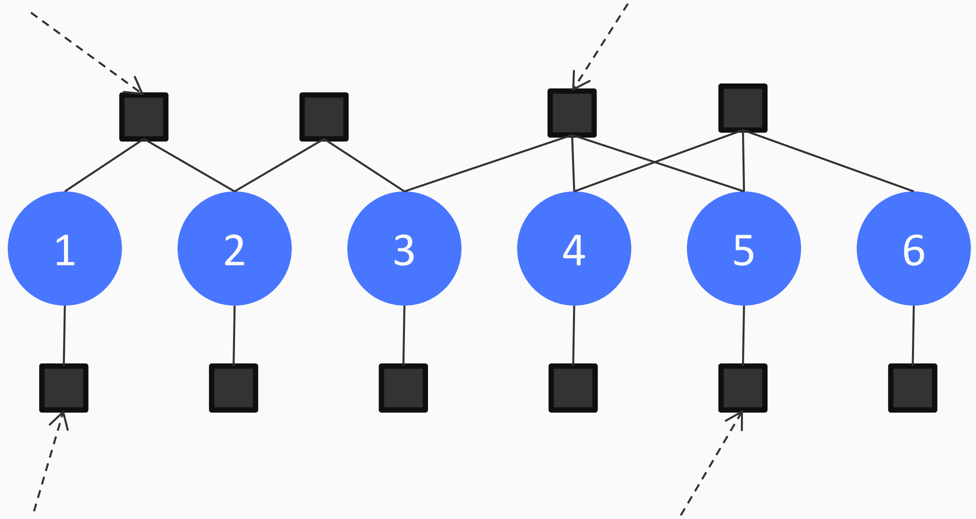

Scores of joint label assignments of variables 1 & 2

Scores of joint label assignments of variables 3, 4 & 5

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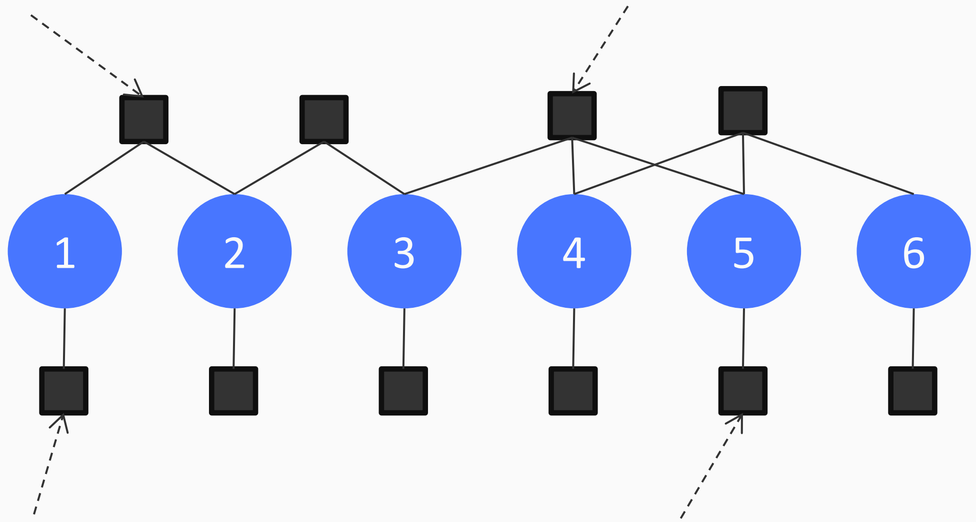
How do we make a joint assignment to these variables that maximizes the total score?



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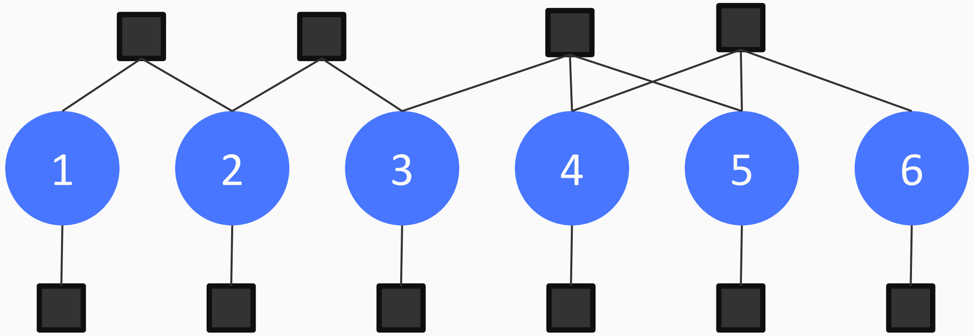
One solution: Traverse a search tree/graph

Suppose we have a “natural” ordering of the variables



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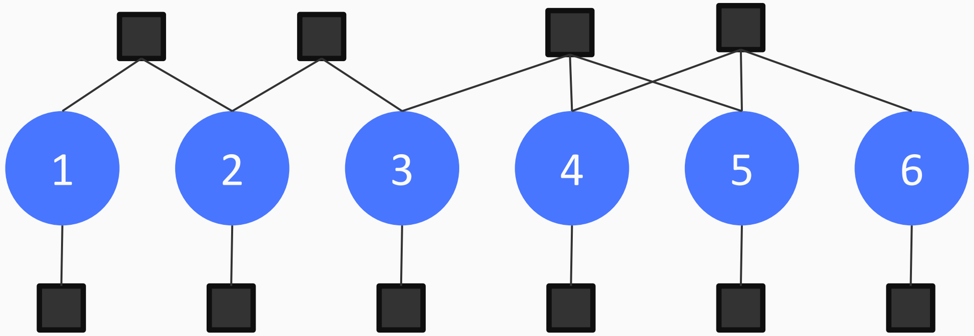

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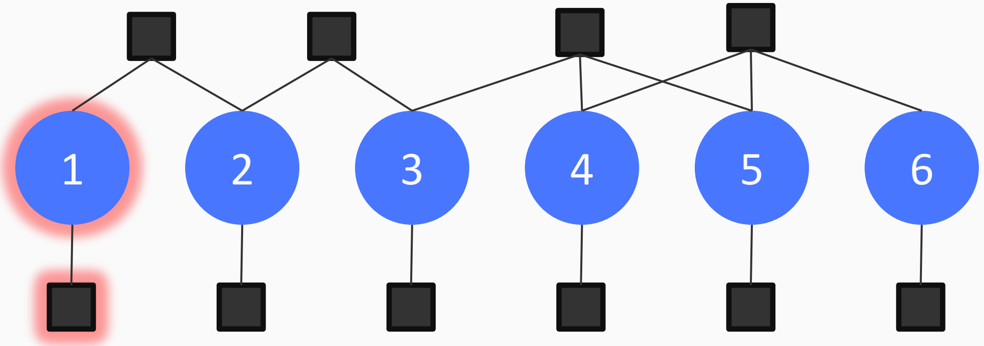

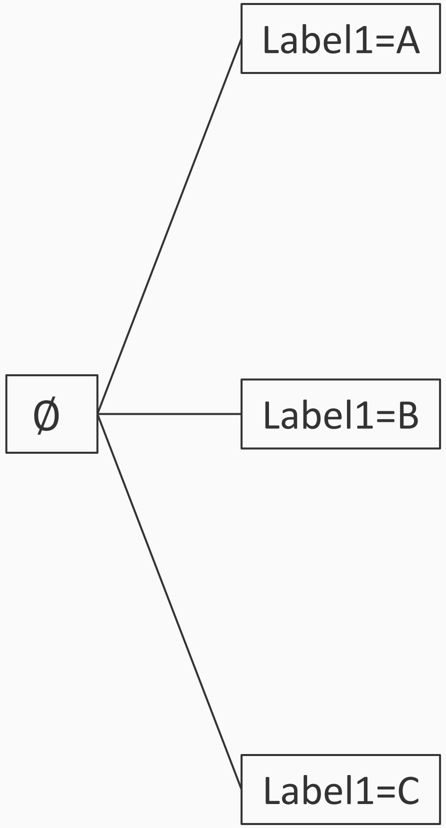

We will assume that there are three possible labels: A, B, C

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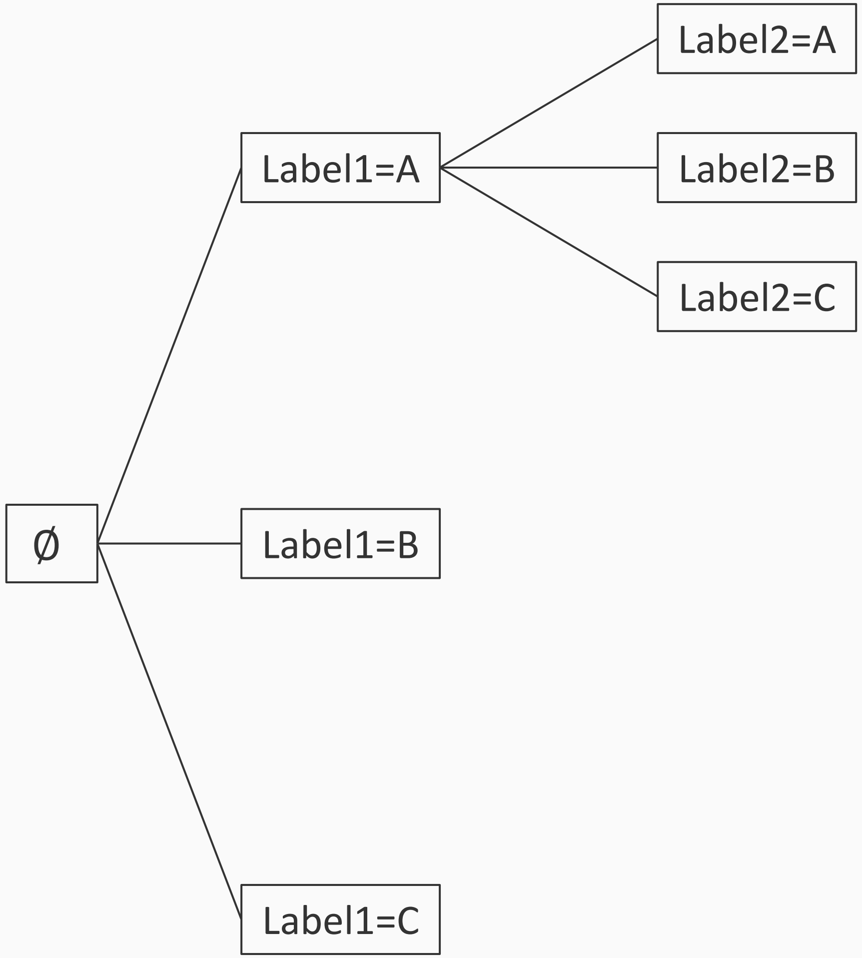

Label2=A

Label1=A

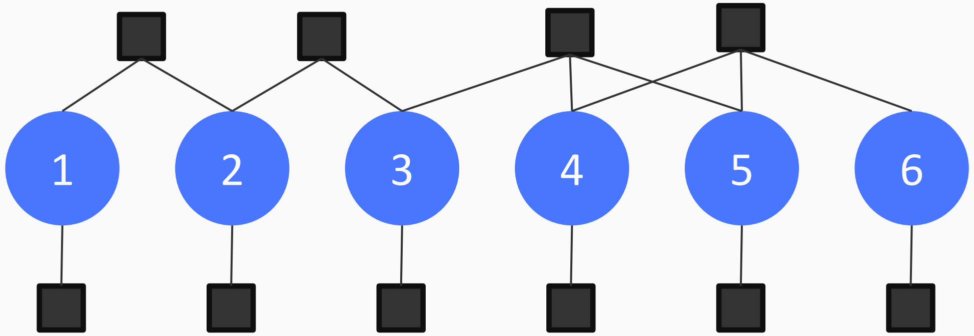
Label2=B

Label2=C

Ø

Label1=B

Label1=C



Given label1=A, we can compute the scores for label2 being A, B, C

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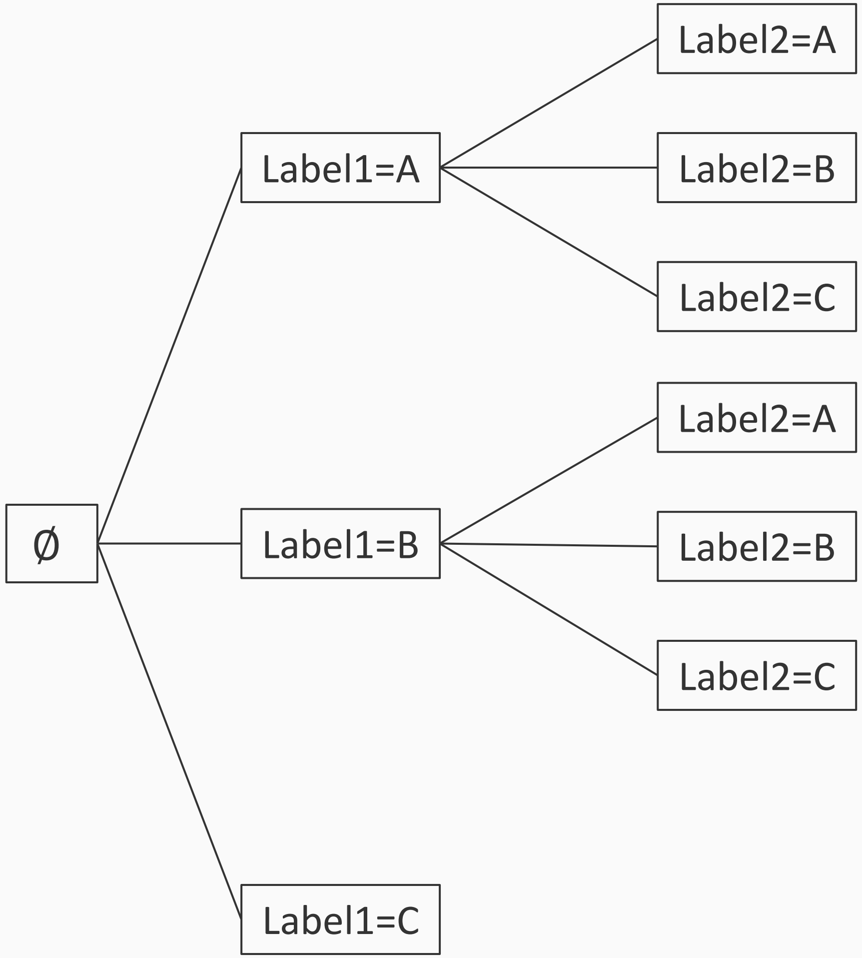
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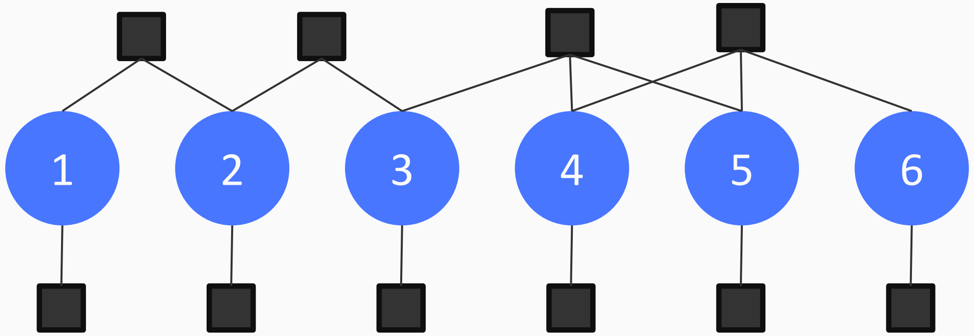

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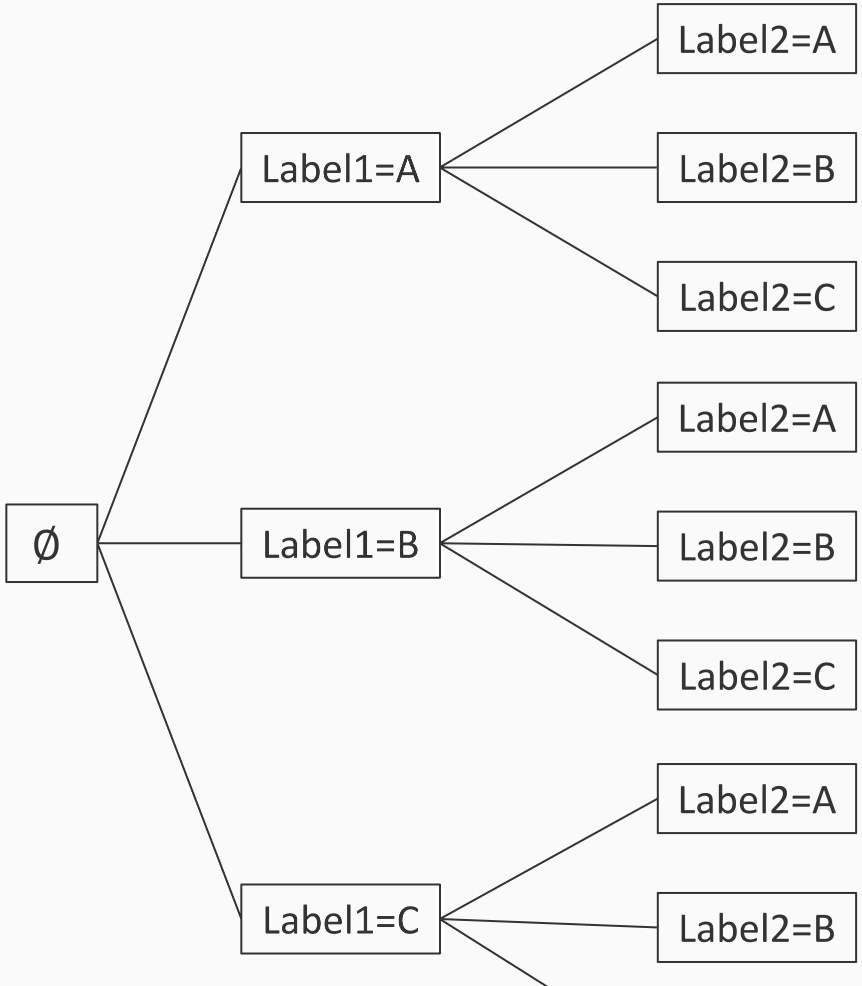

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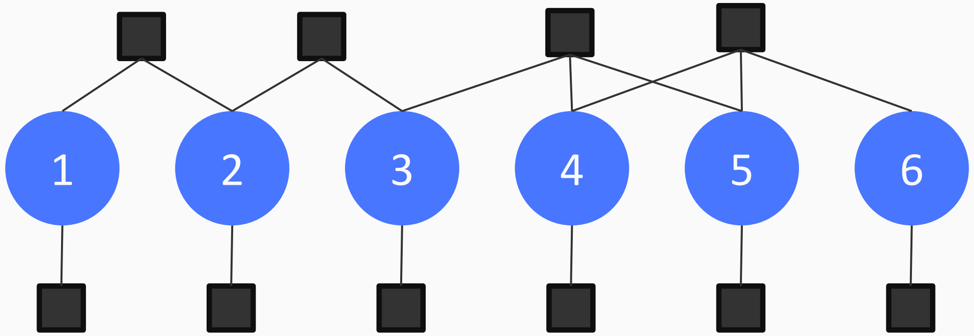

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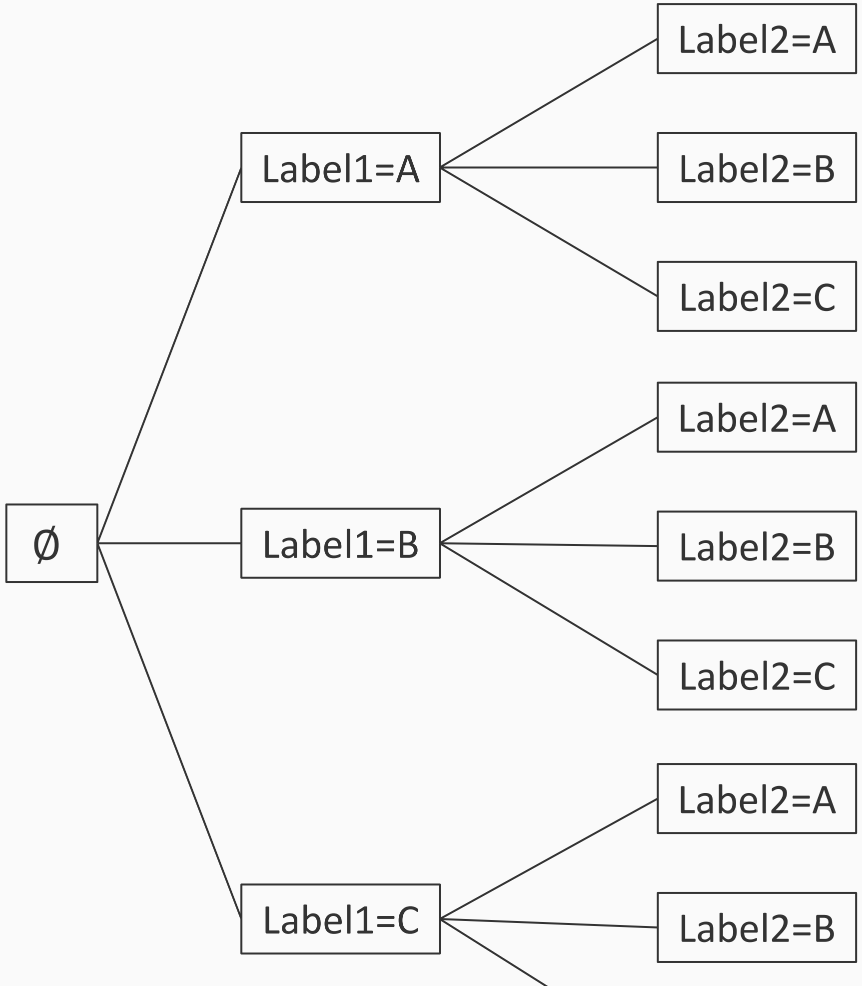

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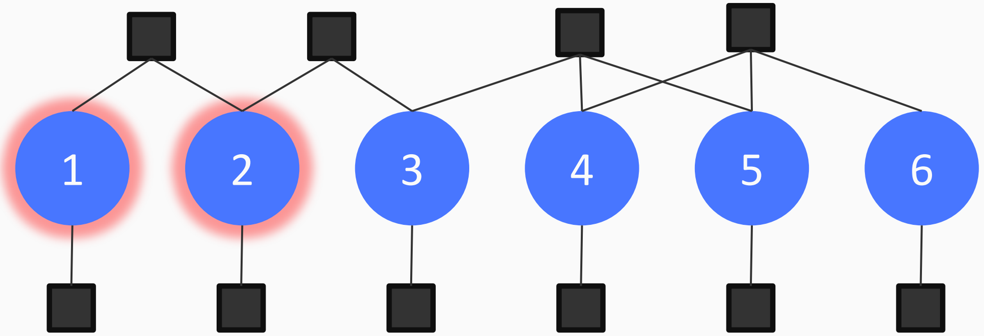

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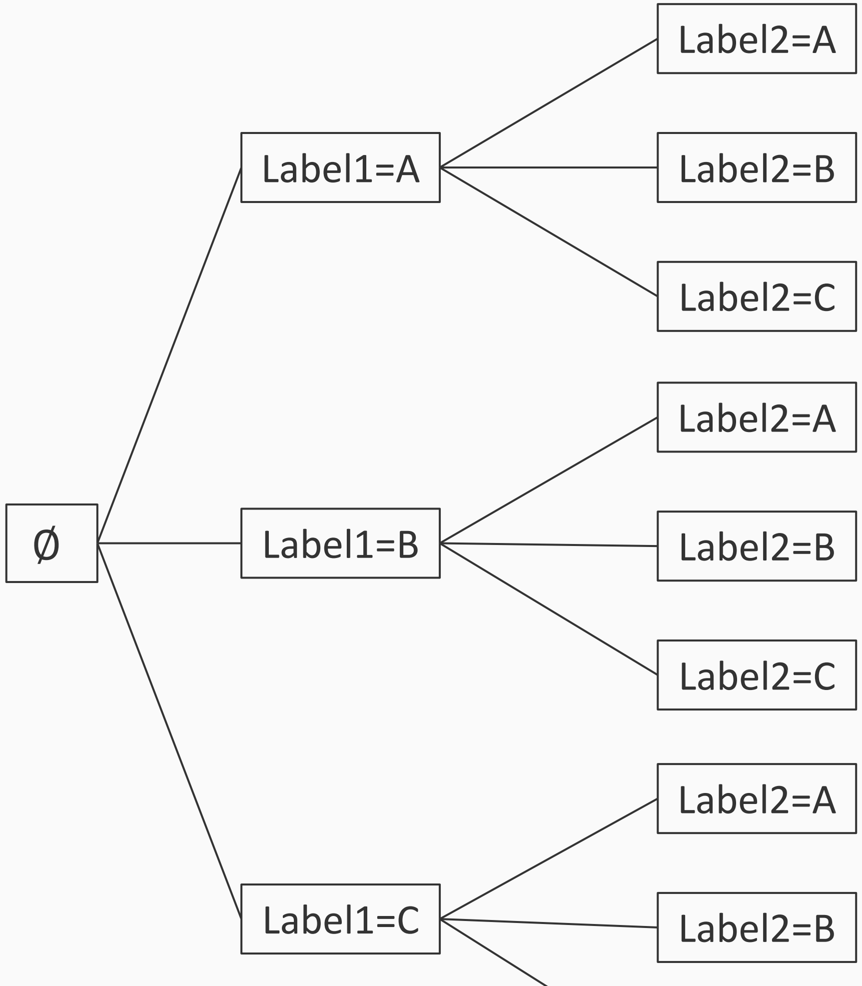

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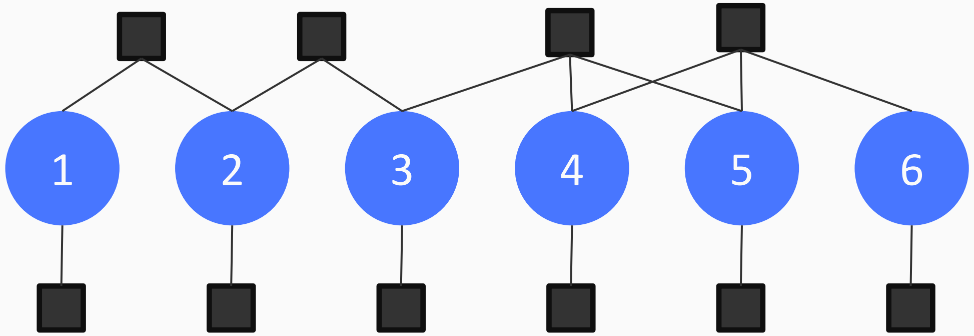

And so on

An example: Decoding with a language model

Given some method to create a probability distribution $P(\mathbf{token} \mid w_0 w_1 w_2 \cdots)$
how should we predict the “best” sequence?

Decoding: The algorithmic question

The answer to this question does not depend on what kind of model we have underneath the probabilities

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What does *best* mean? Ideas?

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What does *best* mean? Ideas?

Some notions of best when it comes to generating text

- Most probable
- Fast
- Does not repeat
- Diverse outputs
- ….

A toy example

Suppose our language model can pick from one of the following words at any step:

a, the, he, she, saw, him, her, apple

Some model predicts a conditional distribution given the words seen so far

Every token in the vocabulary is assigned a probability

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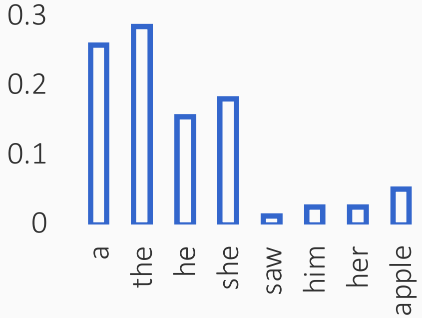

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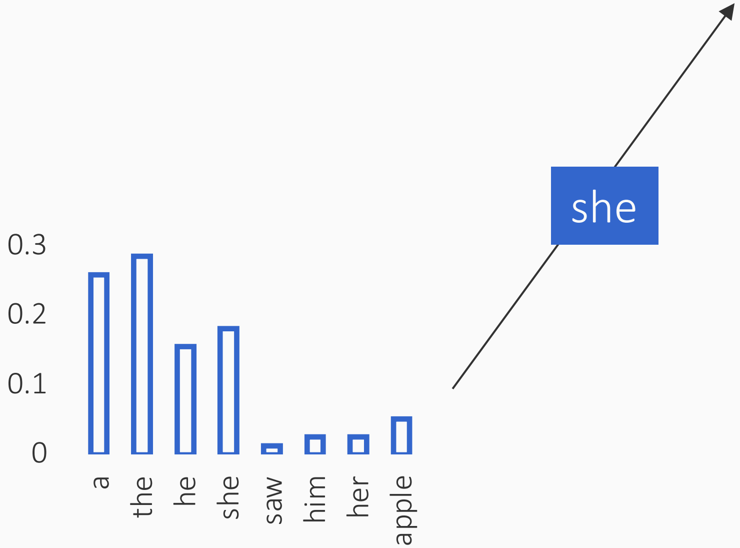

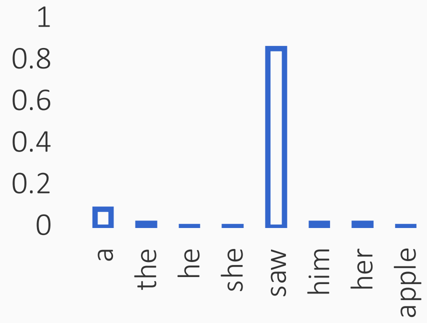

Suppose our decoder decides to pick the word “she”

This produces a new distribution over the next token

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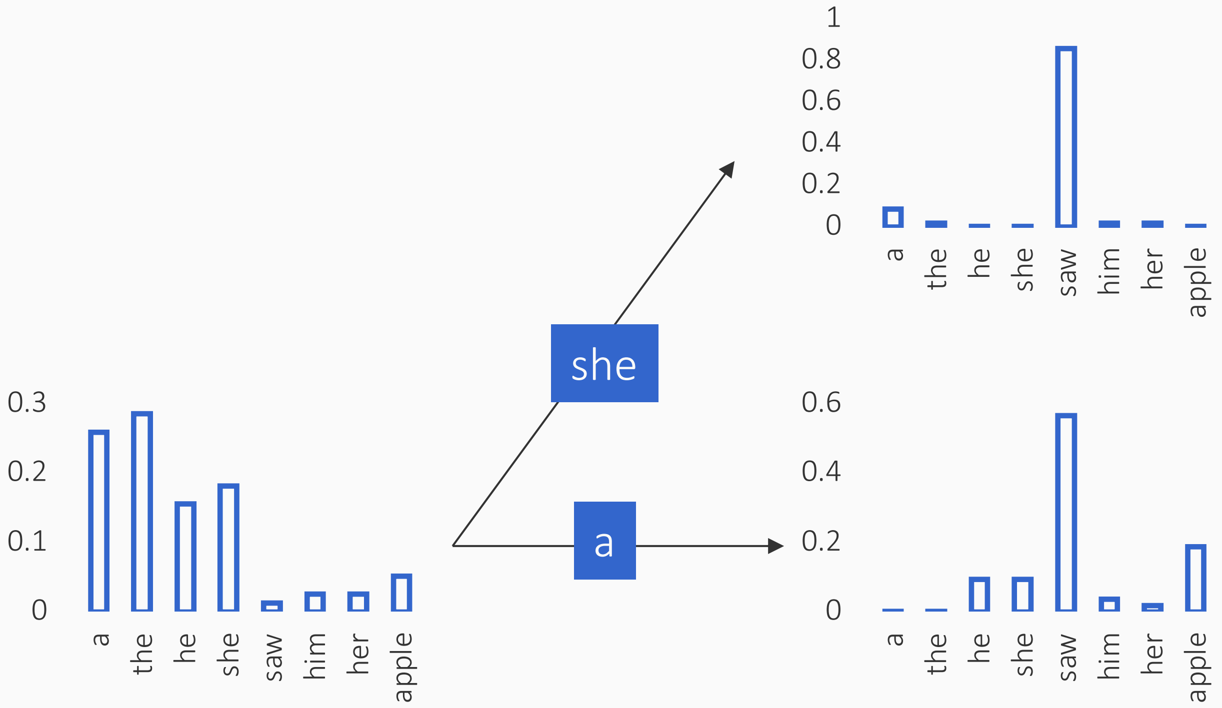

If it picked a different token, say "a", then the next token distribution would be different.

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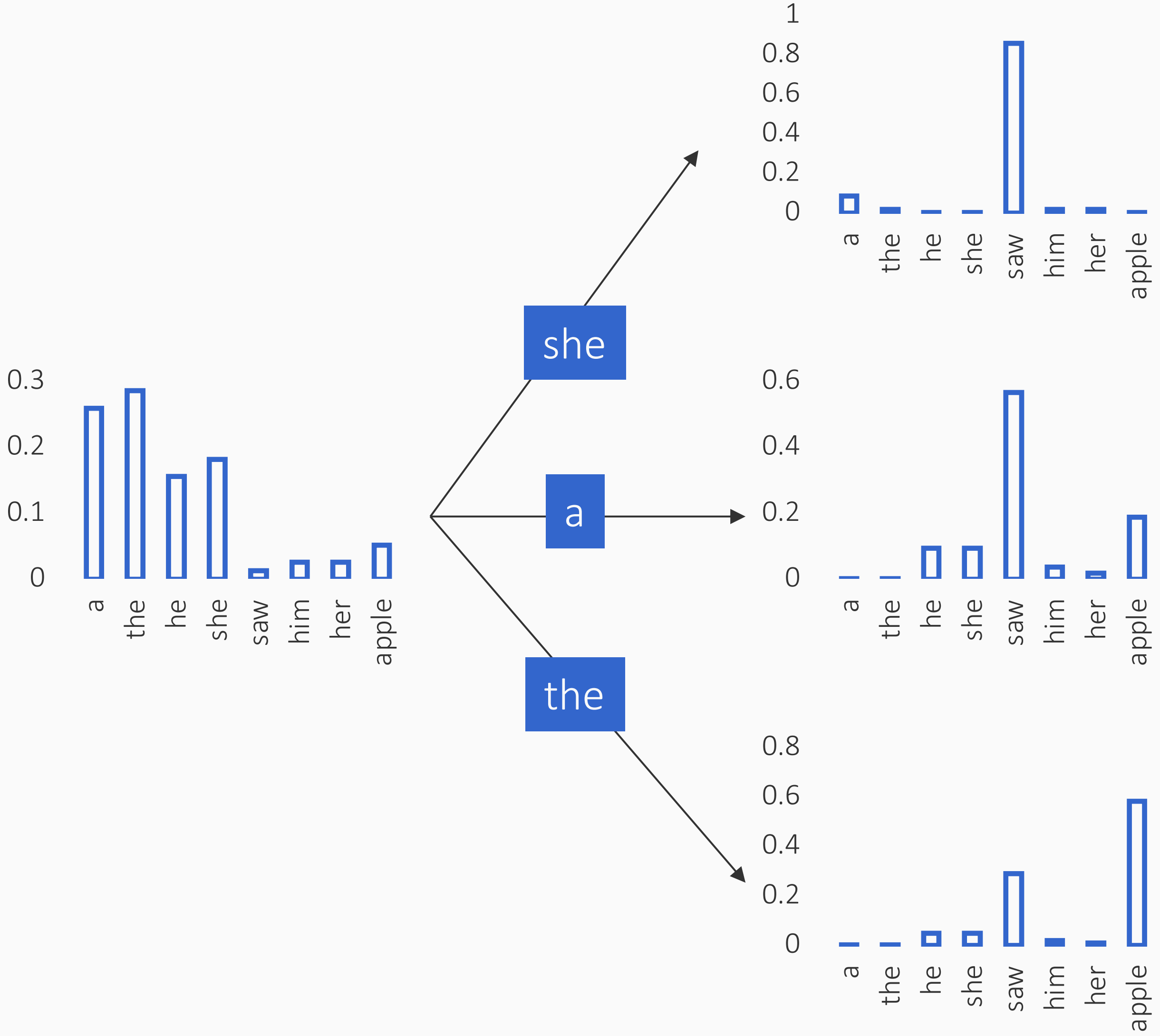

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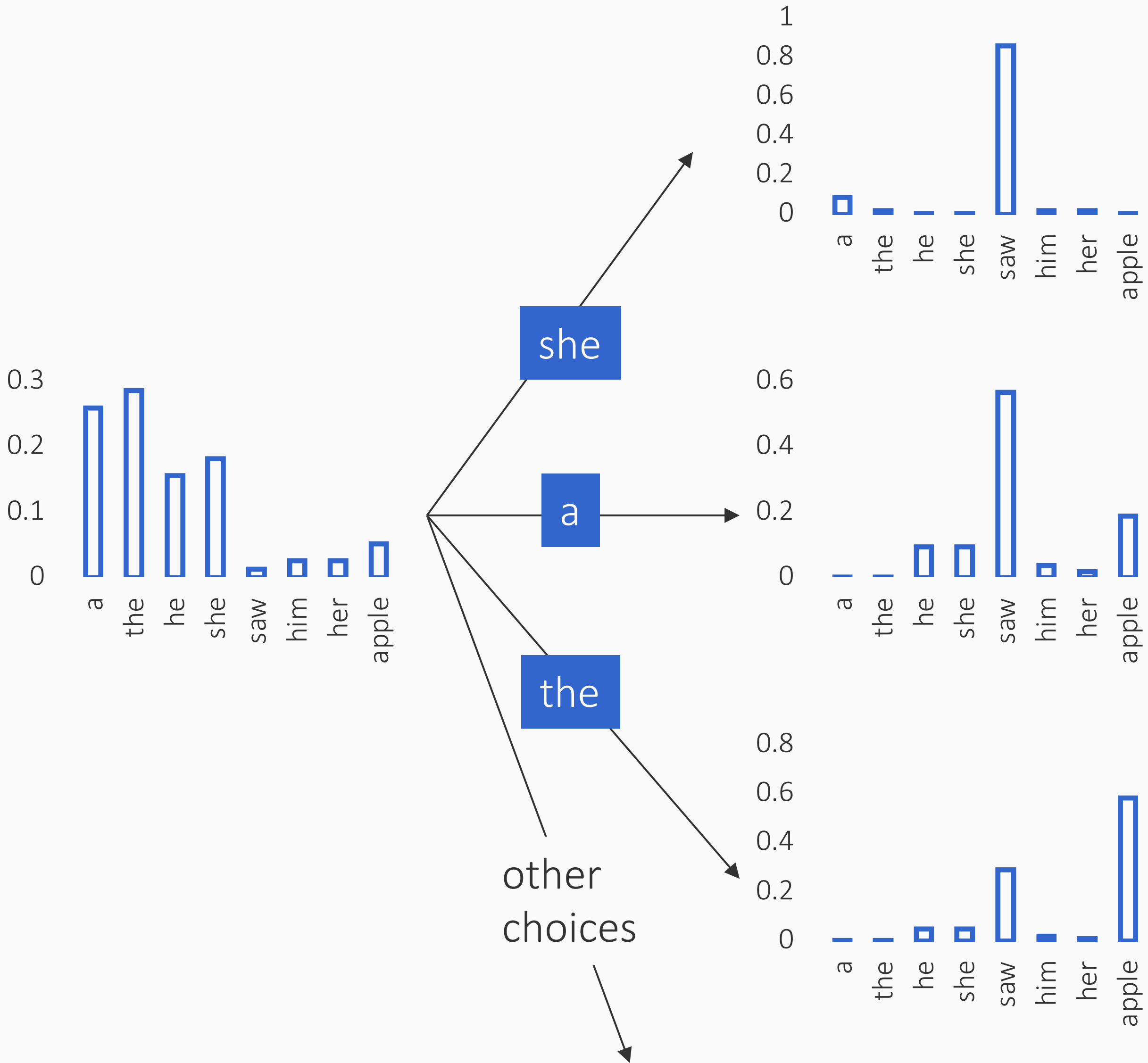

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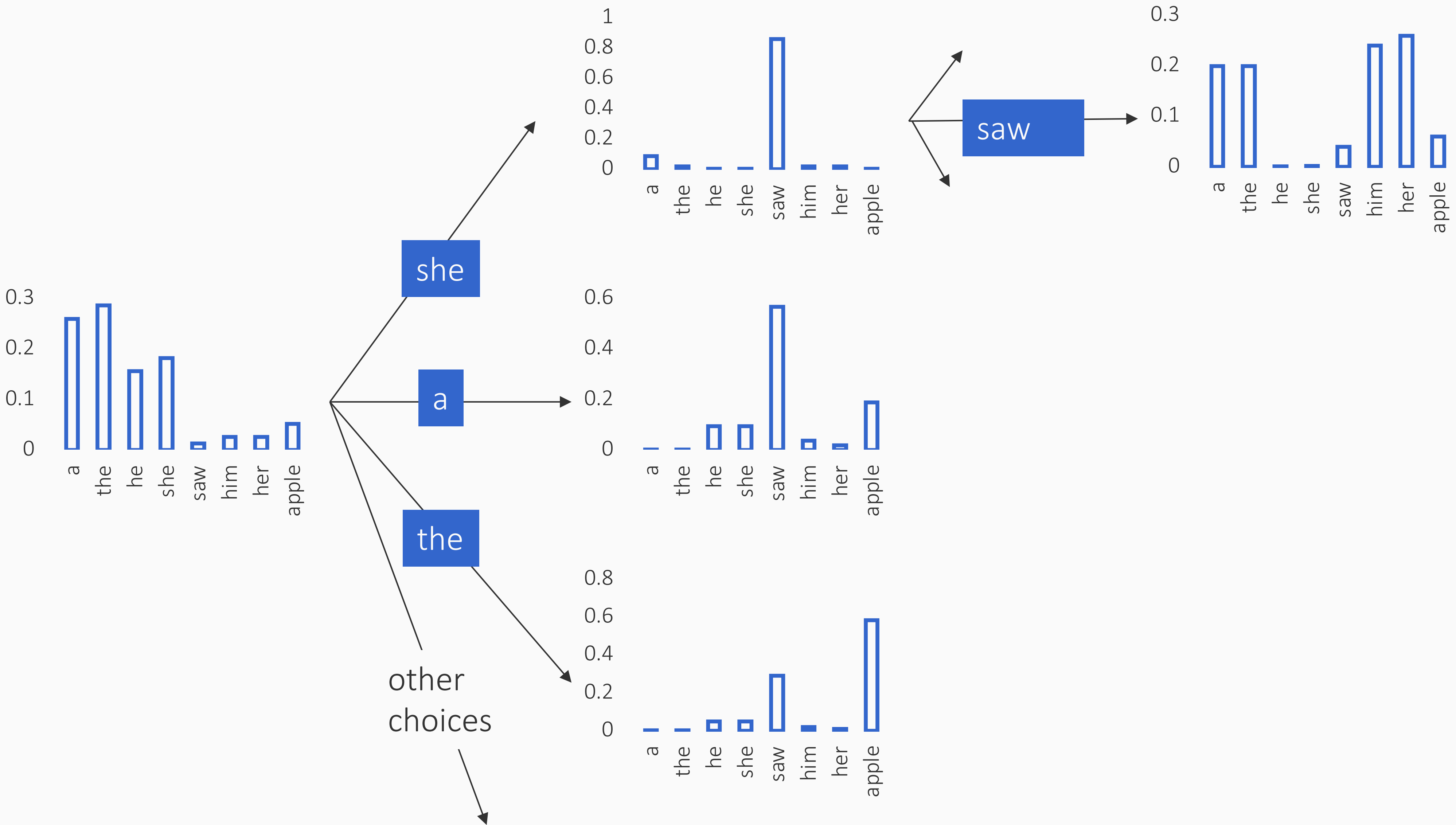

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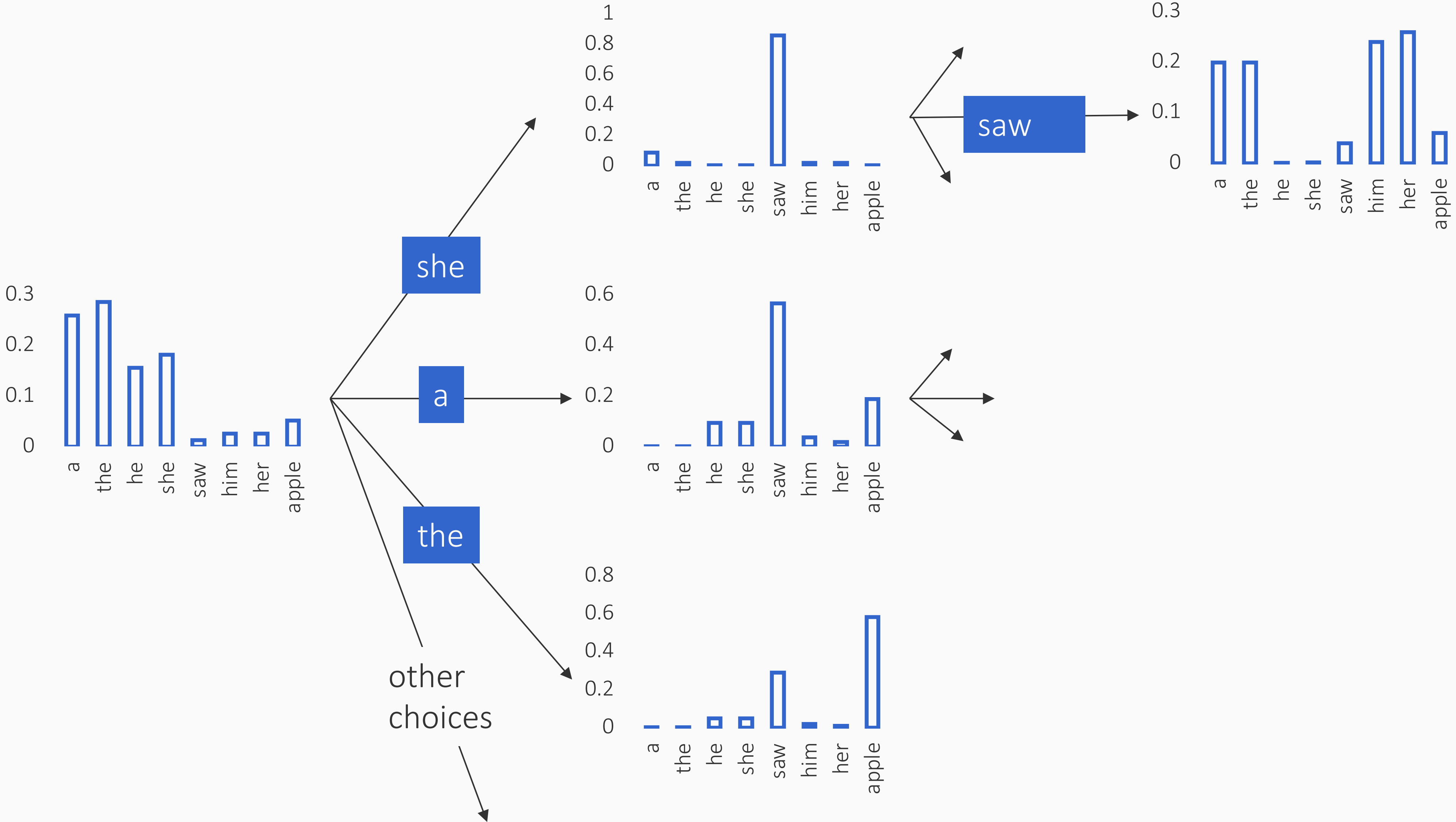

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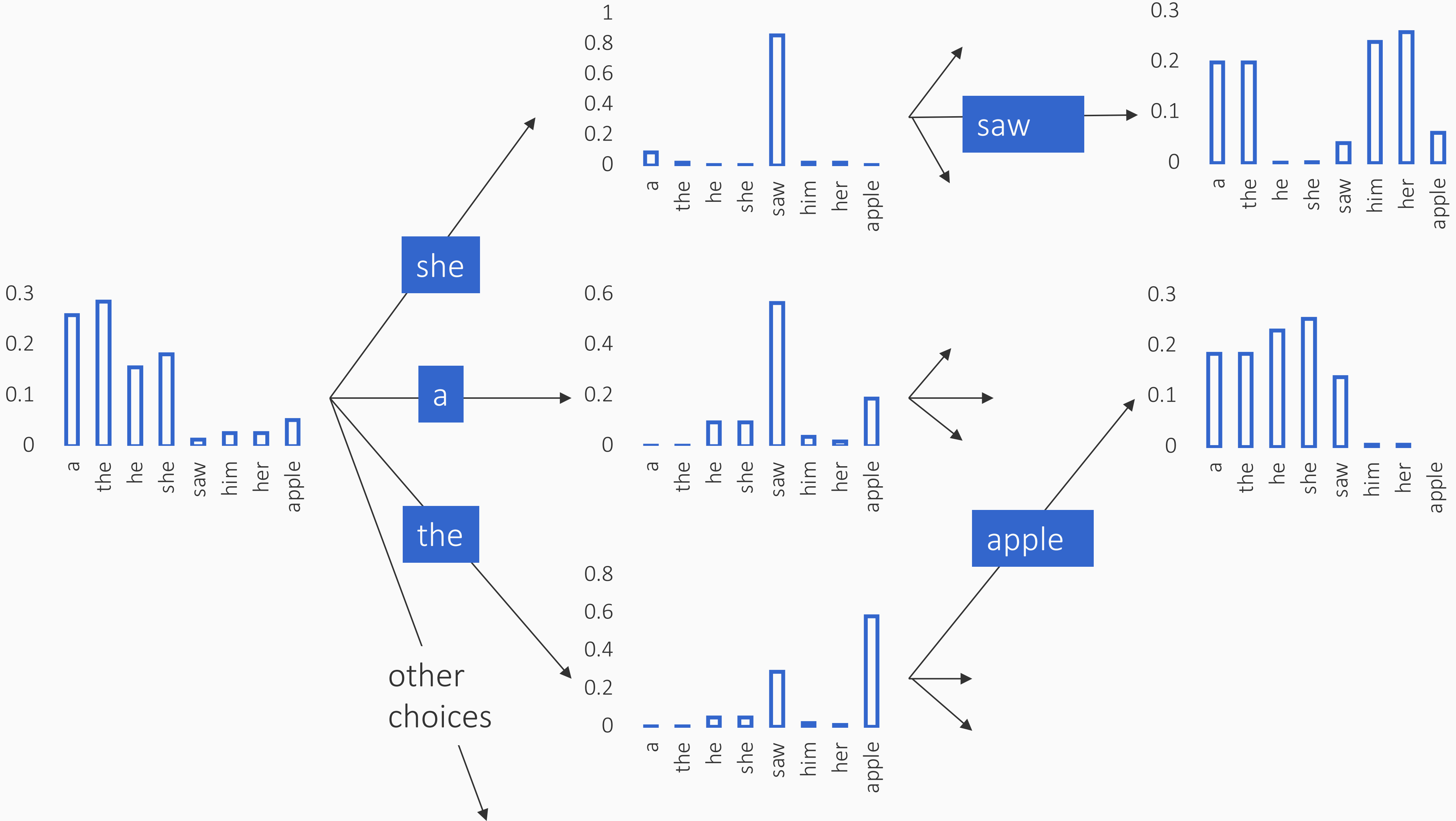

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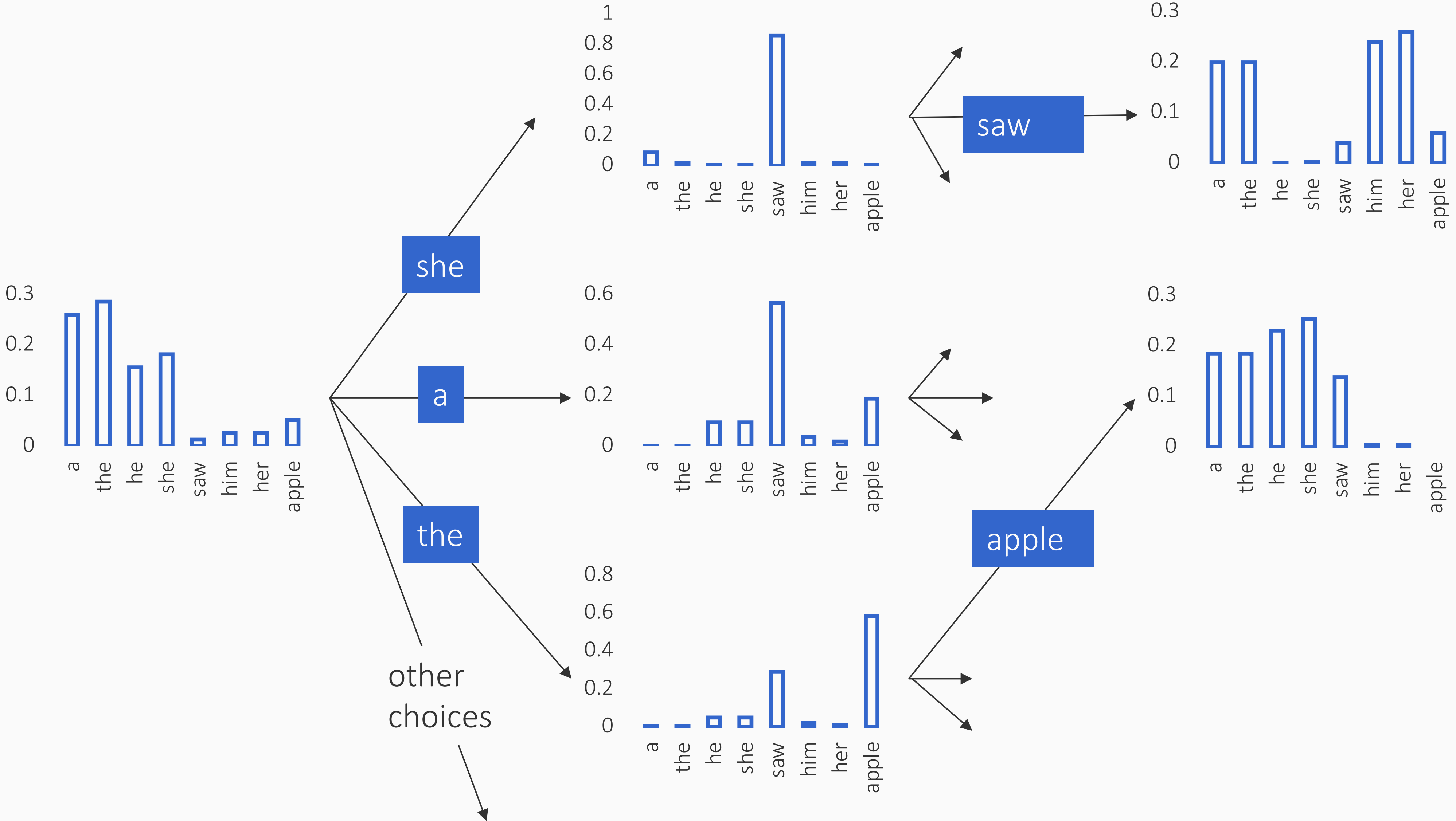


And so on…

Graph algorithms for inference

- Many graph algorithms you have seen are applicable for inference

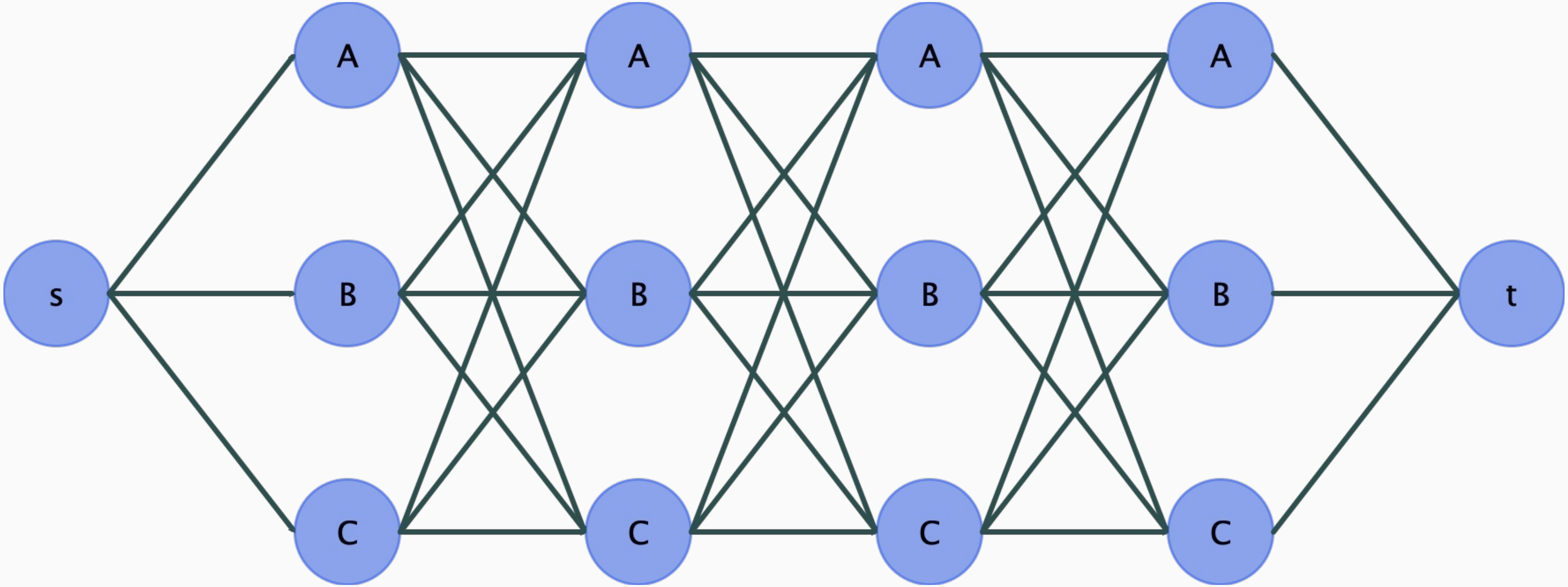
- Some examples
  - “Best” path. Eg: Viterbi, parsing
  - Min-cut/max-flow. Eg: Image segmentation
  - Maximum spanning tree. Eg: Dependency parsing
  - Bipartite matching. Eg: Aligning sequences

Best path for inference

- Broad description of approach:
  - Construct a graph/hypergraph from the input and output
  - Decompose the total score along edge/hyperedges
  - Inference is finding the shortest/longest path in this weighted graph

Example: The Viterbi algorithm finds a shortest path in a specific graph

Viterbi algorithm as best path



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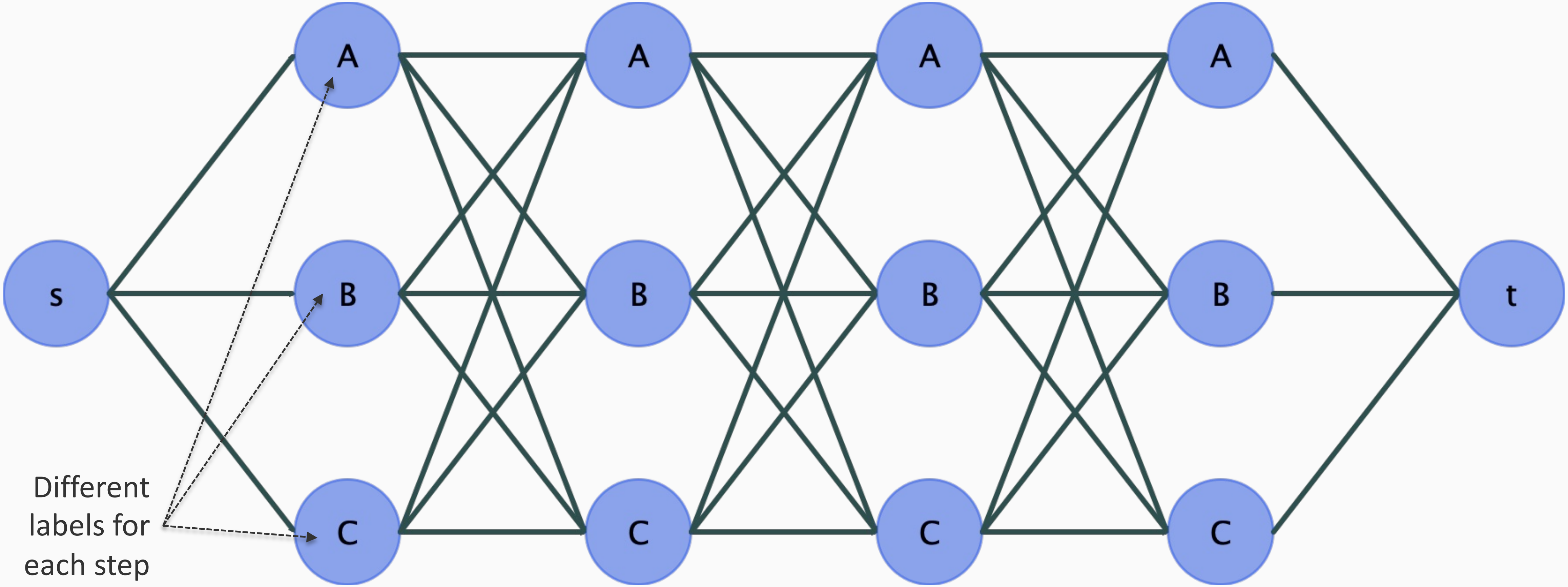
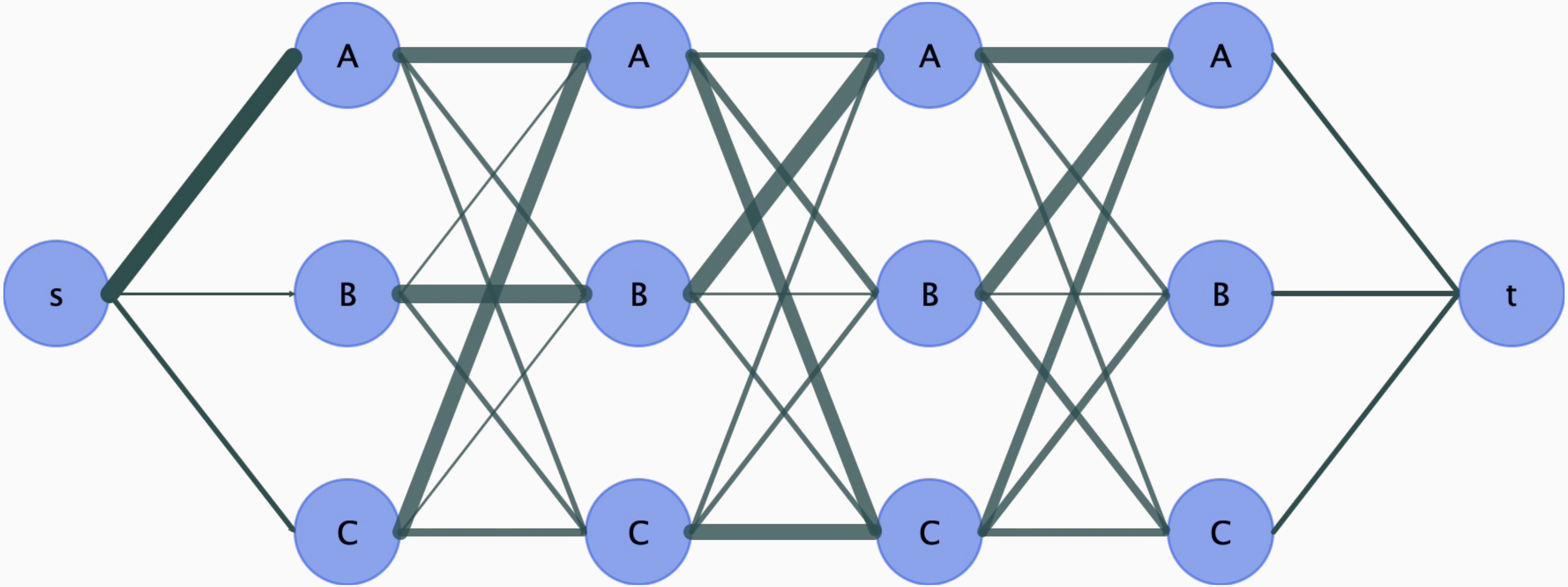


Different labels for each step

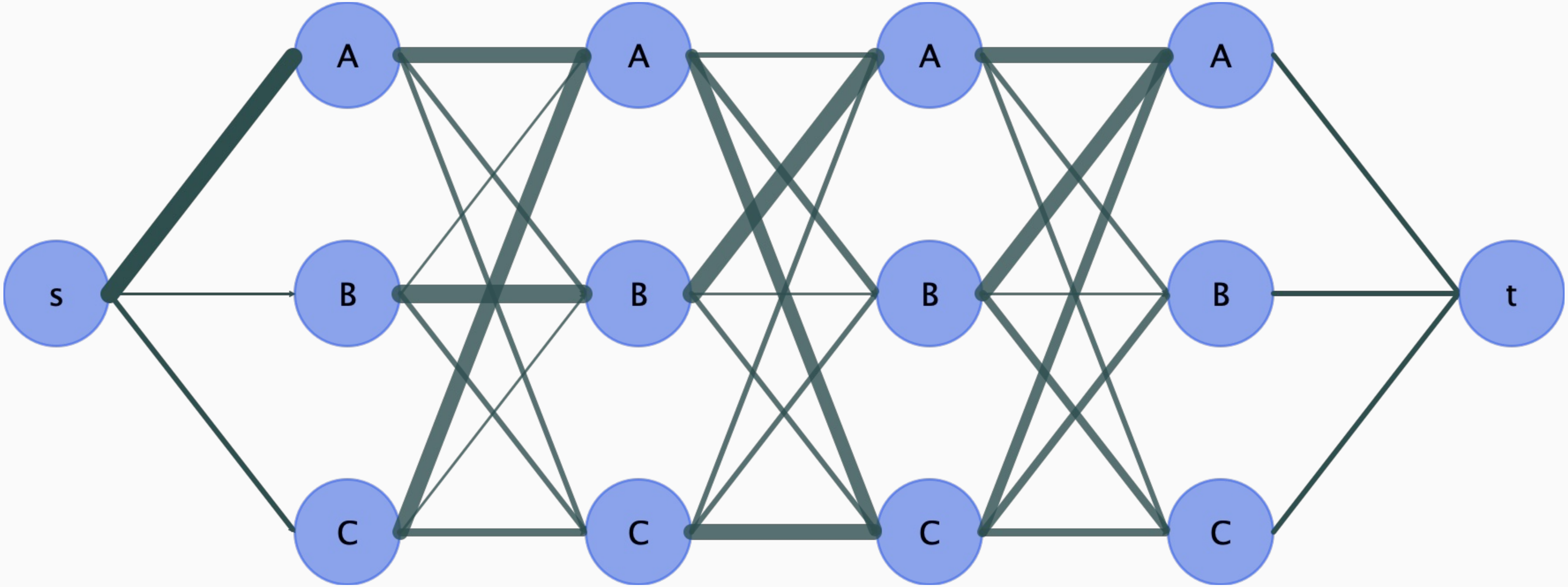
Viterbi algorithm as best path

Each edge has a weight associated with it



Viterbi algorithm as best path

Goal: To find the highest scoring path in this trellis



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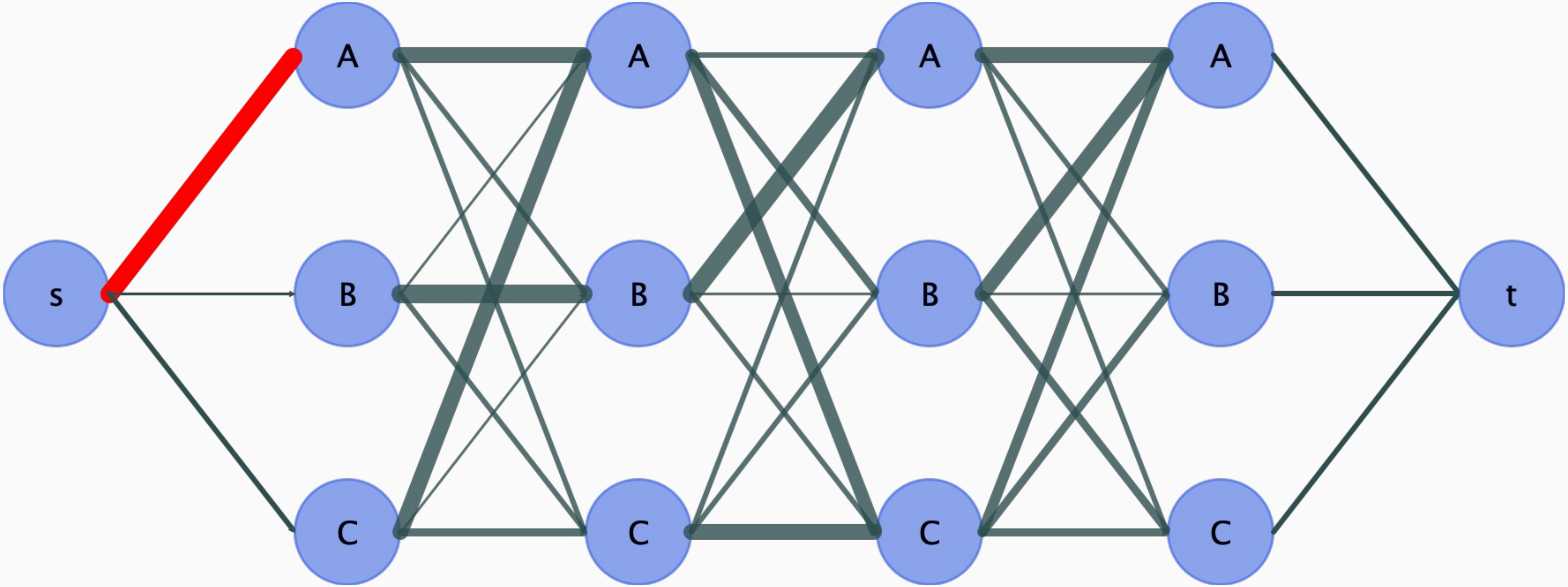

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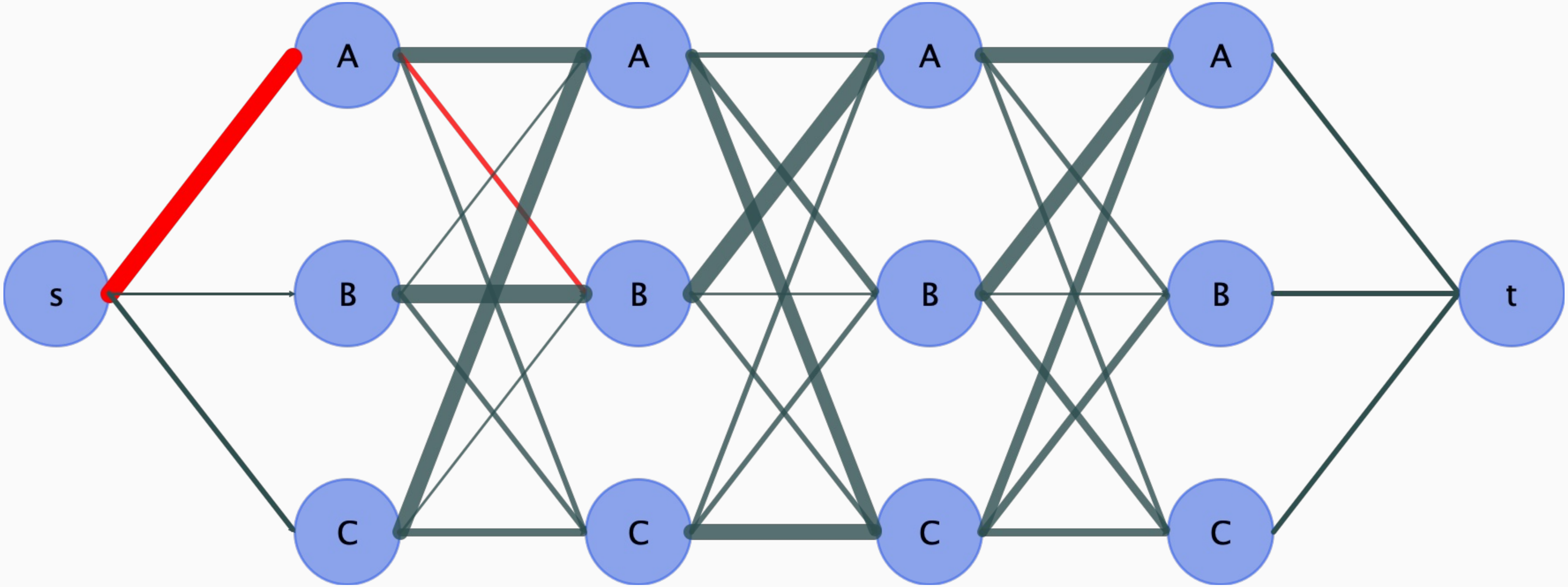

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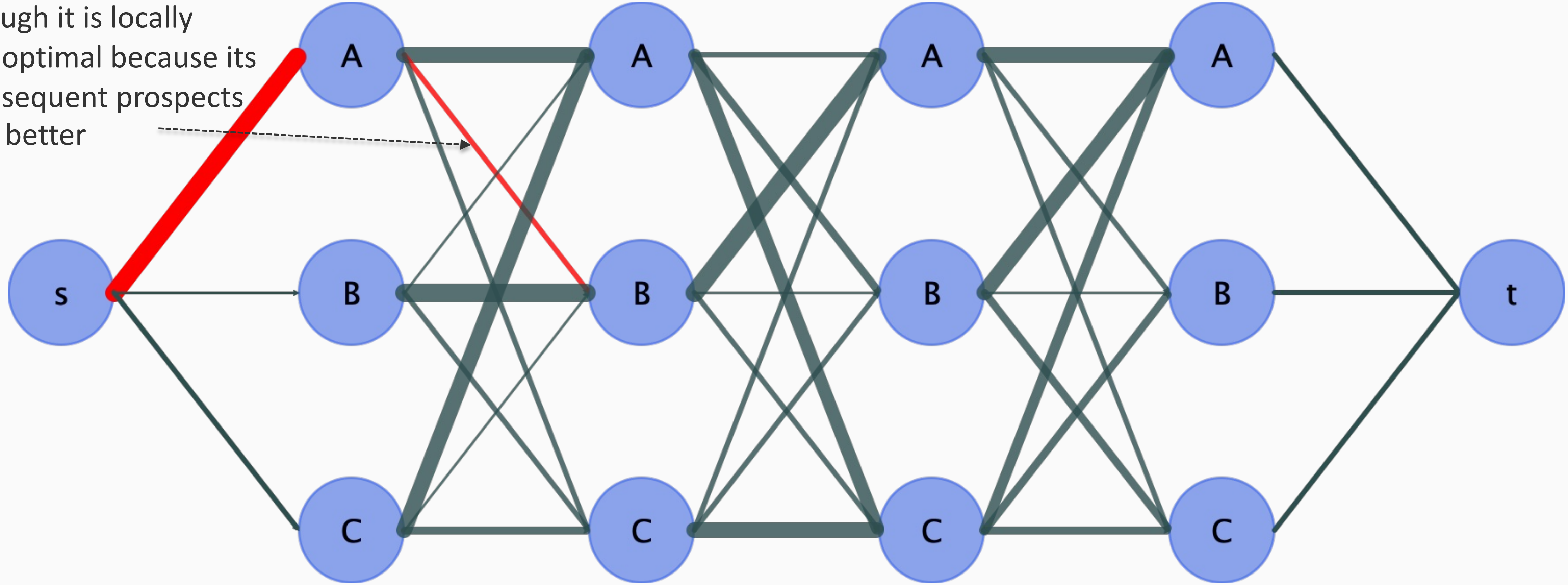

This edge is chosen even though it is locally suboptimal because its subsequent prospects are better

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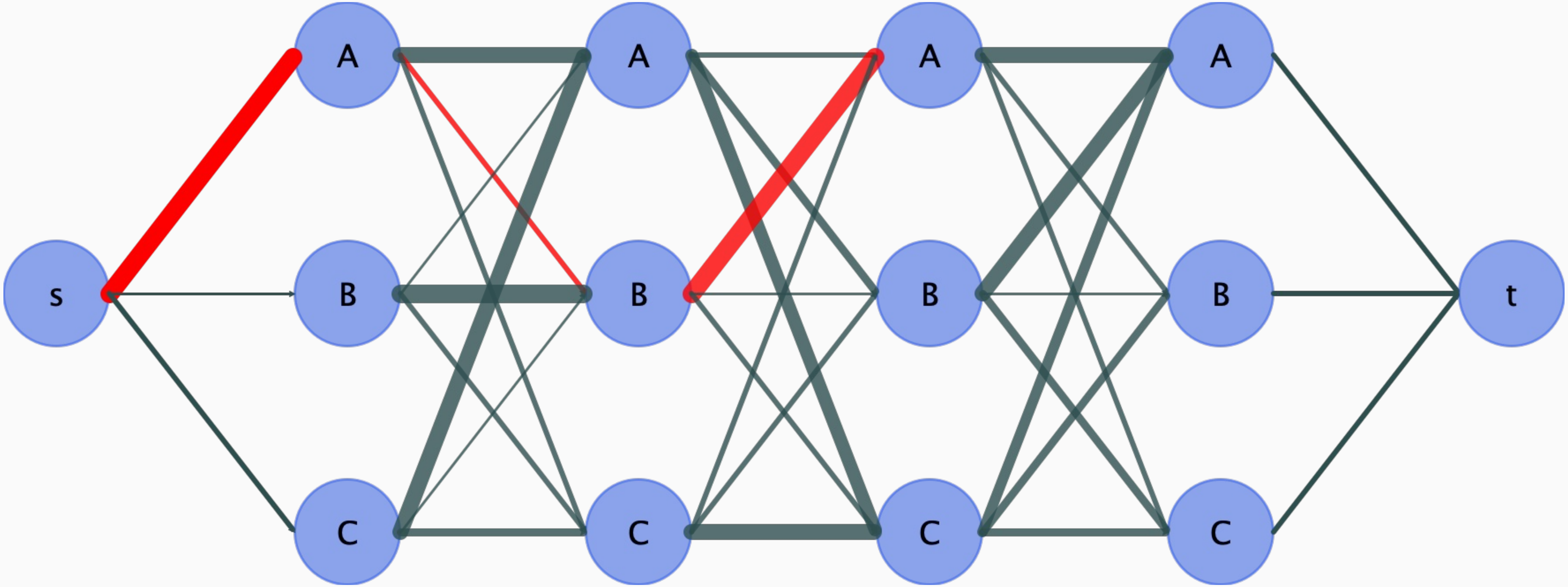

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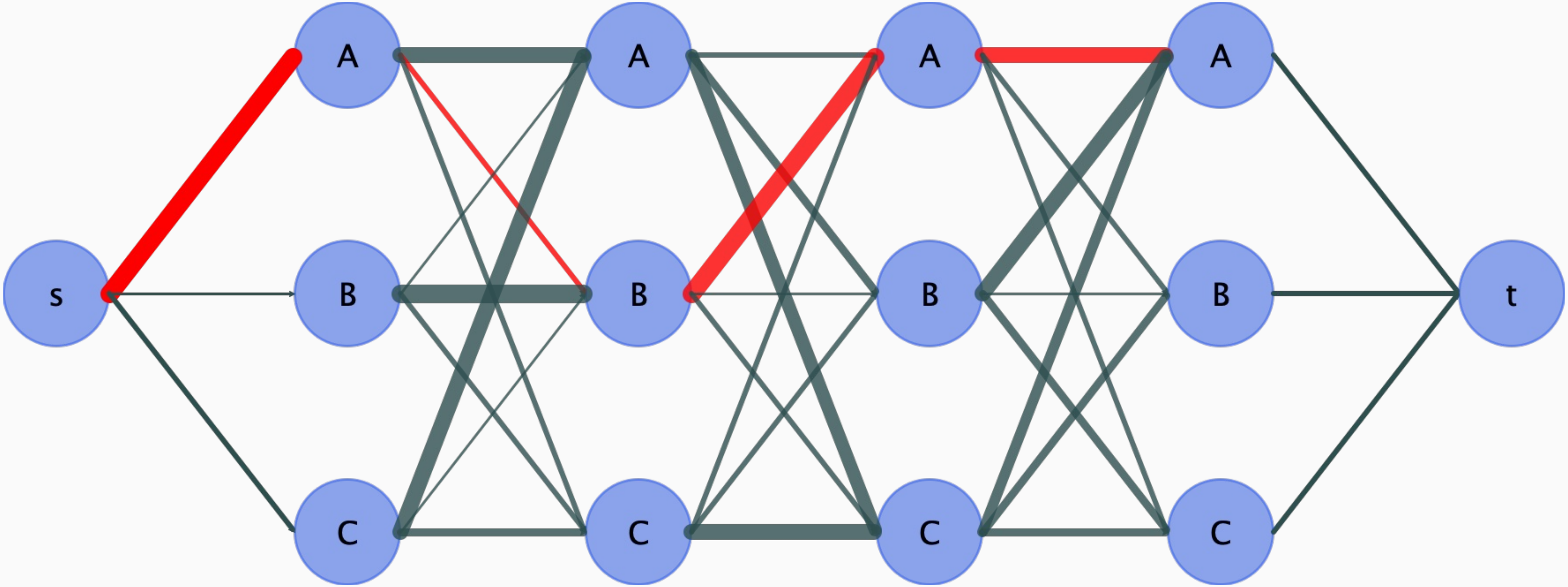

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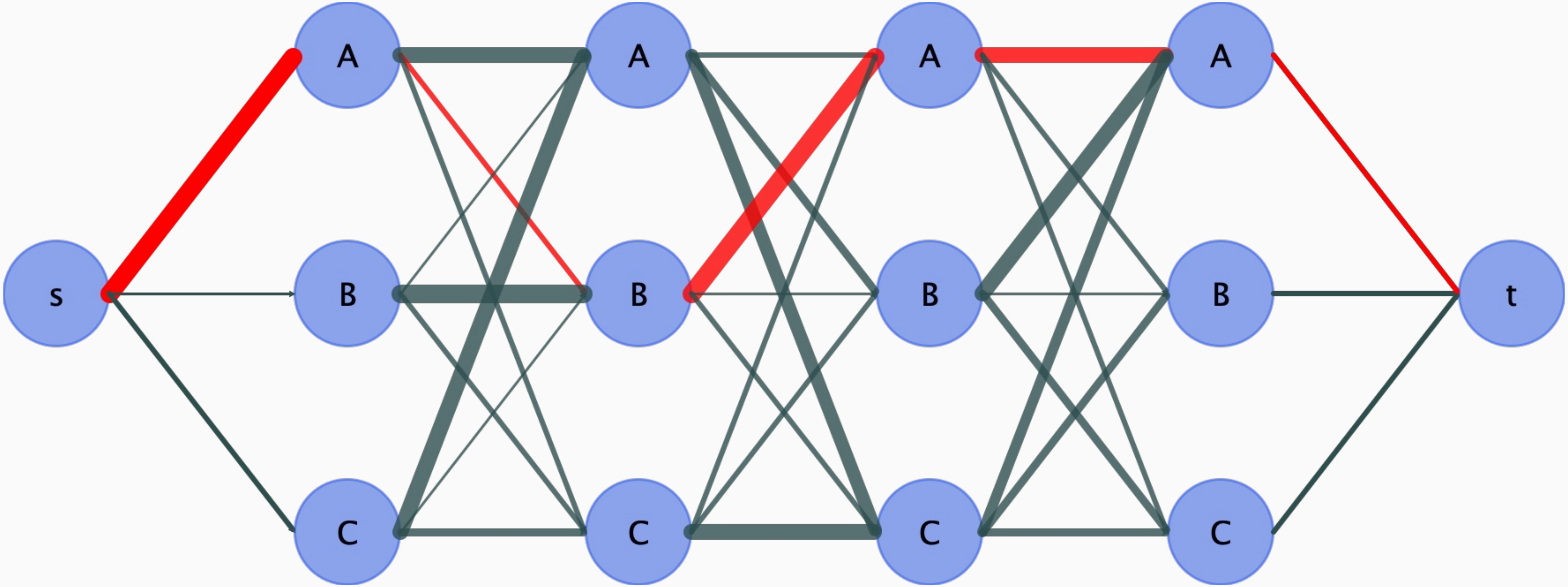

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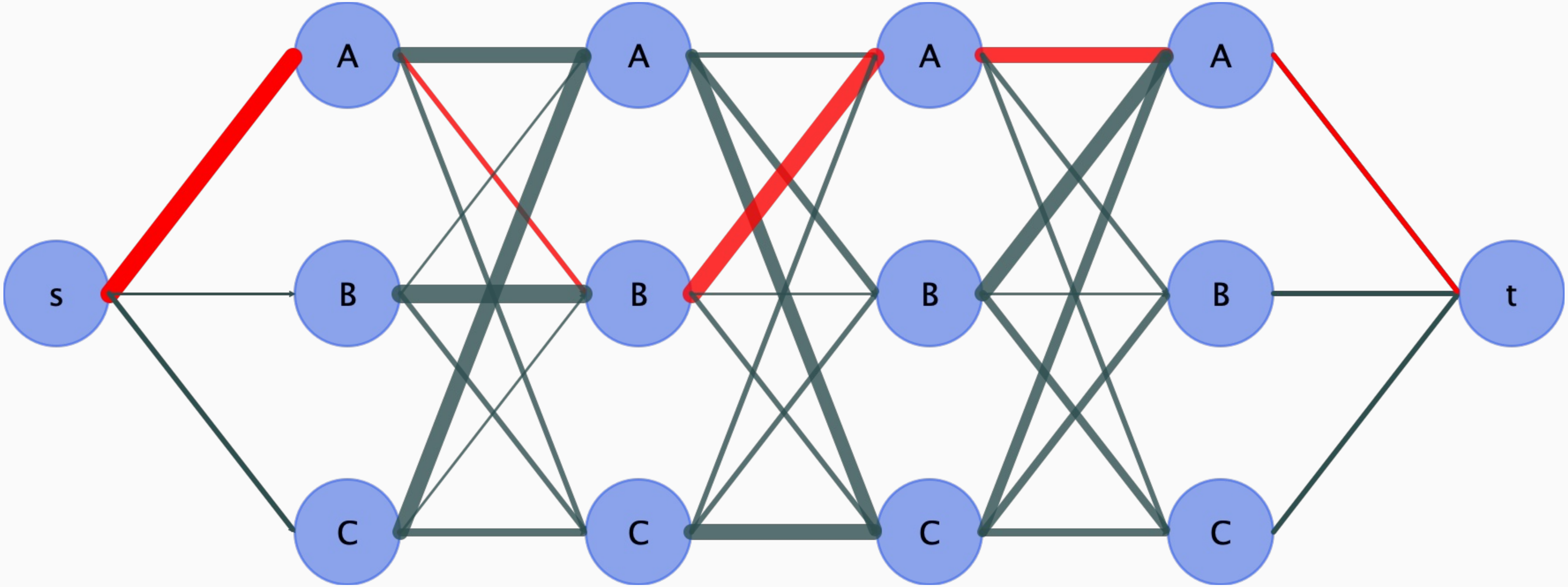


No cycles
Nodes and edges have a specific meaning
Ordering helps

Best path algorithms

- Dijkstra’s algorithm
  - Cost functions should be non-negative

- Bellman-ford algorithm
  - Slower than Dijkstra’s algorithm but works with negative weights

- A* search
  - If you have a heuristic that gives the future path cost from a state but does not over-estimate it

Dynamic programming

- General solution strategy for inference

- Examples
  - Viterbi, CKY algorithm, Dijkstra’s algorithm, and many more

- Key ideas:
  - Memoization: Don’t re-compute something you already have
  - Requires an ordering of the variables

- Remember:
  - The hypergraph may not allow for the best ordering of the variables
  - Existence of a dynamic programming algorithm does not mean polynomial time/space.
    - State space may be too big. Use heuristics such as beam search

Inference as search: Setting

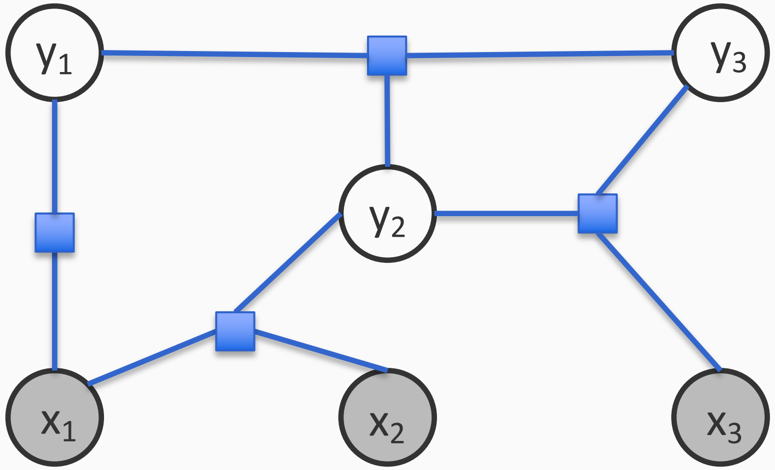
- Predicting a graph as a sequence of decisions

- Data structures:
  - State: Encodes partial assignment to the variables
  - Transitions: Move from one partial assignment to another
  - Start state
  - End state: We have a full assignment
    - There may be more than one end state

- Each transition is scored with the learned model

- Goal: Find an end state that has the highest total score

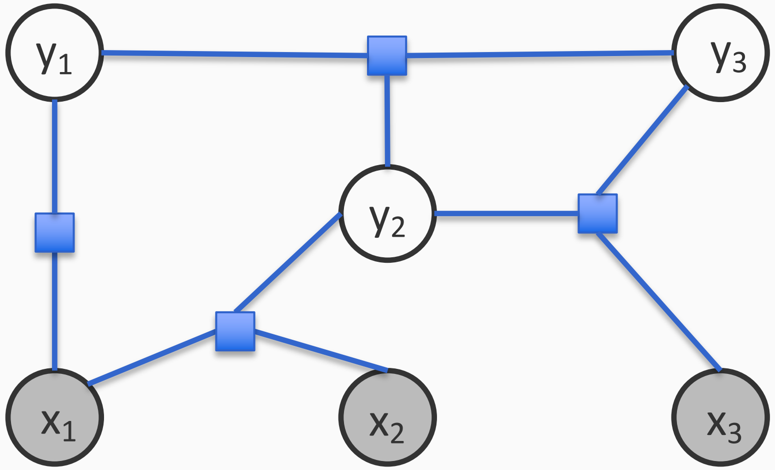
Example



Suppose each y can be one of A, B or C

- State: Triples (y_1, y_2, y_3) all possibly unknown
  - (A, -, -), (-, A, A), (-, -, -),…
- Transition: Fill in one of the unknowns
- Start state: (-,-,-)
- End state: All three y's are assigned

Example



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Start state: No assignments

(-,-,-)

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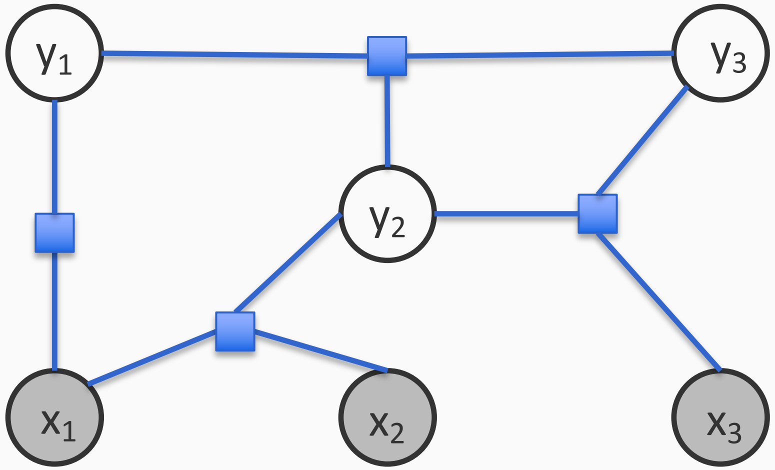

Suppose each y can be one of A, B or C

- State: Triples (y_1, y_2, y_3) all possibly unknown
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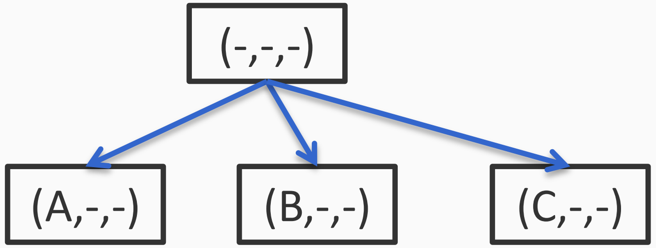
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(A,-,-)

(B,-,-)

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Fill in a label in a slot. The edge is scored by the factors that can be computed so far

Example

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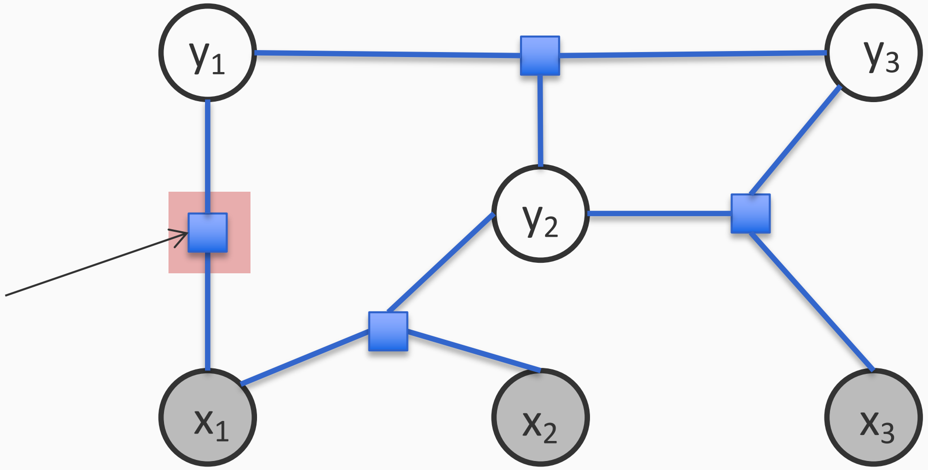

The only score that can be computed if we only know the value of y_1

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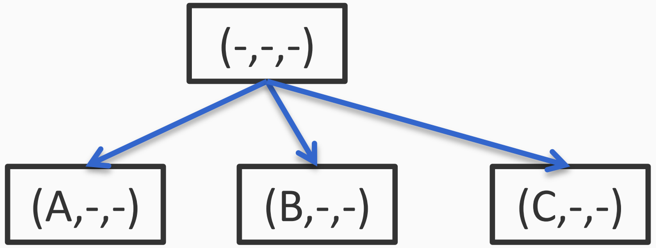
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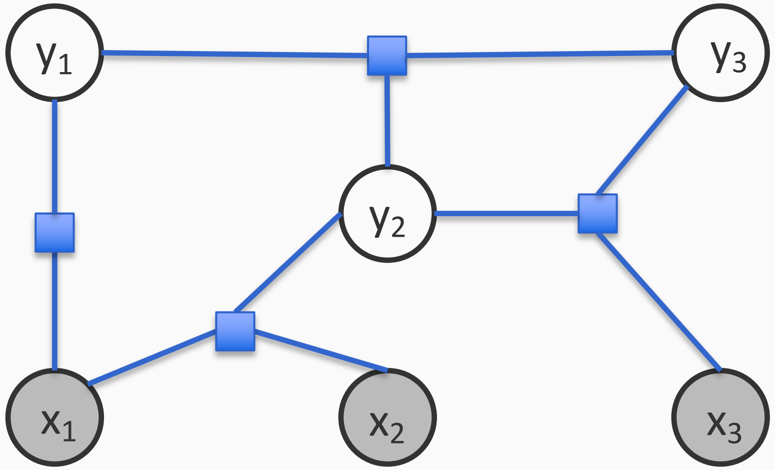

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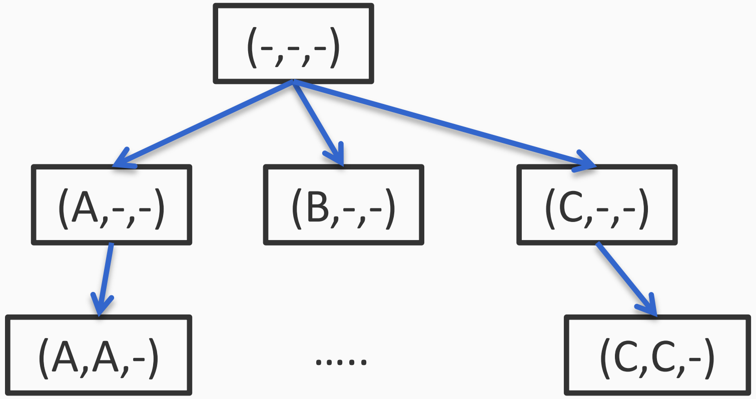

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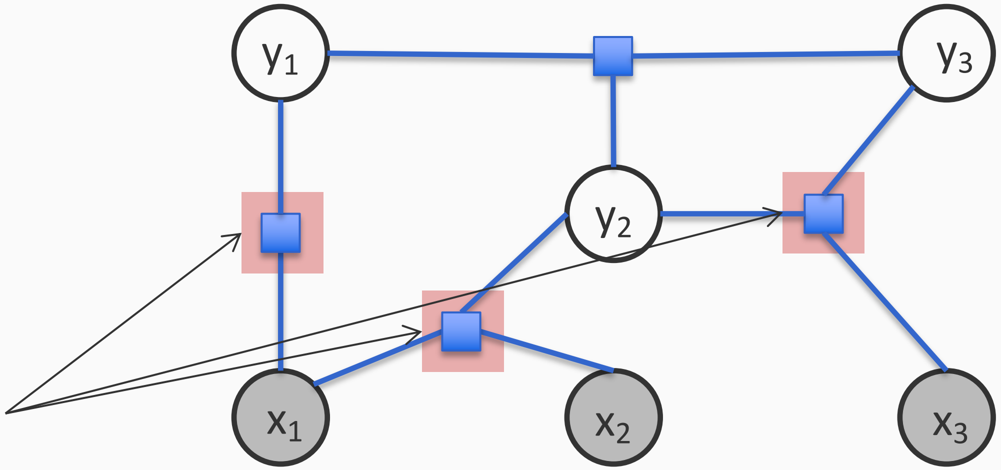
Keep assigning values to slots

Example

Suppose each y can be one of A, B or C



The scores that can be computed if we only know the values of y_1 and y_2

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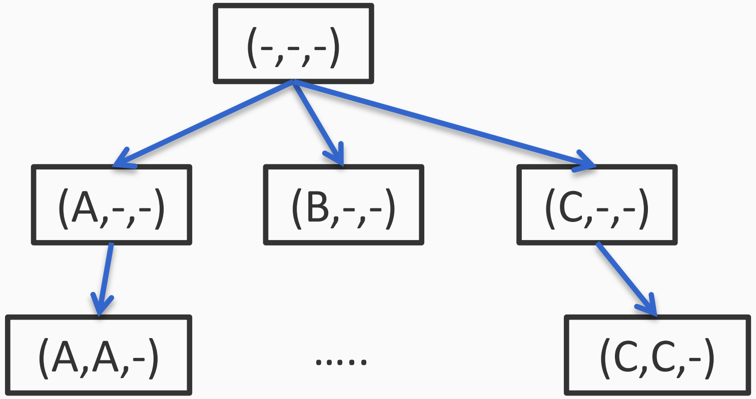

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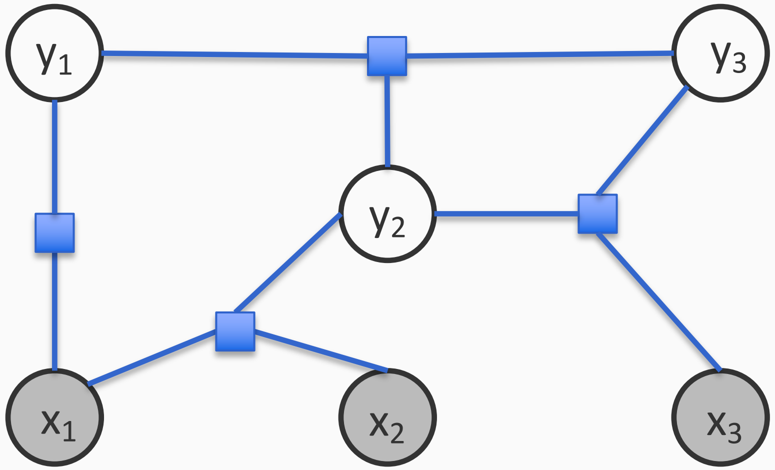

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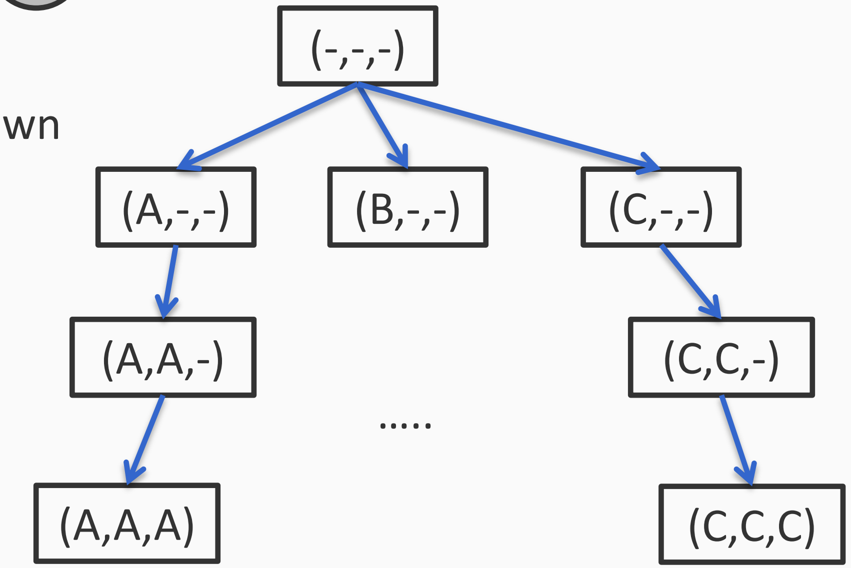
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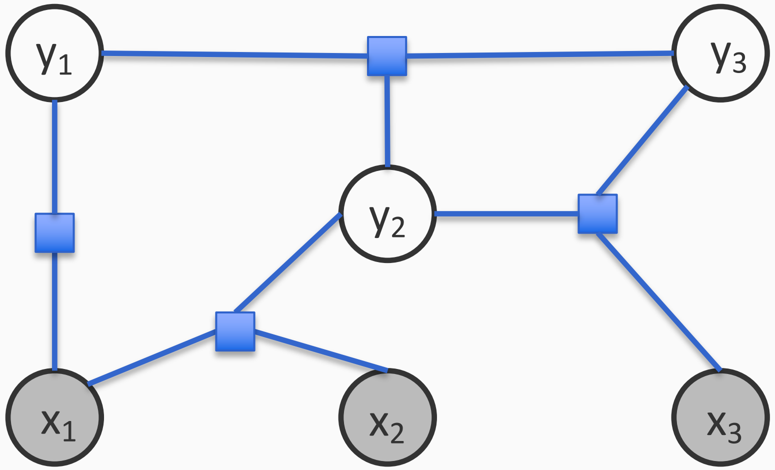
(A,A,-) ….. (C,C,-)

(A,A,A) (C,C,C)

Till we reach a goal state

Example



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Note: Here we have assumed an ordering (y_1, y_2, y_3)

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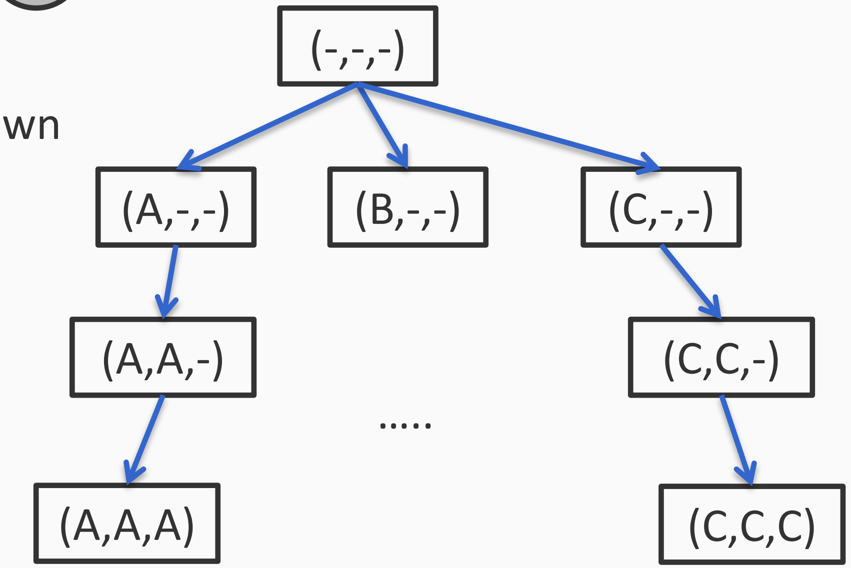
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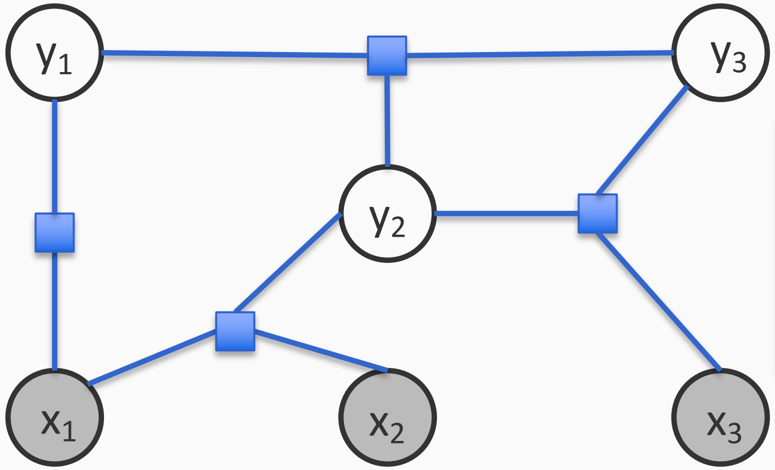

Suppose each y can be one of A, B or C

The goal of inference: To traverse this graph from the start state and reach the end state that has the best (highest/lowest) score

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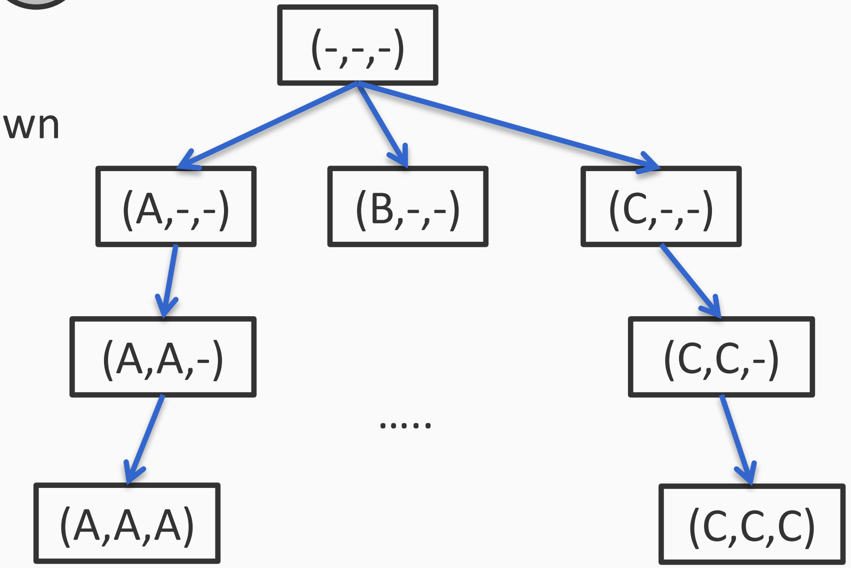

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(B,-,-)
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(C,C,-)

…..

(A,A,A)
(C,C,C)

Graph search algorithms

- Standard graph search algorithms can be used for inference

- Breadth/depth first search
  - Keep a stack/queue/priority queue of “open” states
    - That is, states that are to be explored

  - The good: Guaranteed to be correct
    - Explores every option

  - The bad?
    - Explores every option: Memory is an issue
    - Could be slow for any non-trivial graph

Different decoding strategies exist

Search based decoding

Sampling based decoding

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Deterministic approaches that involves searching the space of sequences to select one

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Deterministic approaches that involves searching the space of sequences to select one

- Greedy decoding
- Beam search

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- Random sampling
- Top-K sampling
- Nucleus sampling

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Greedy search

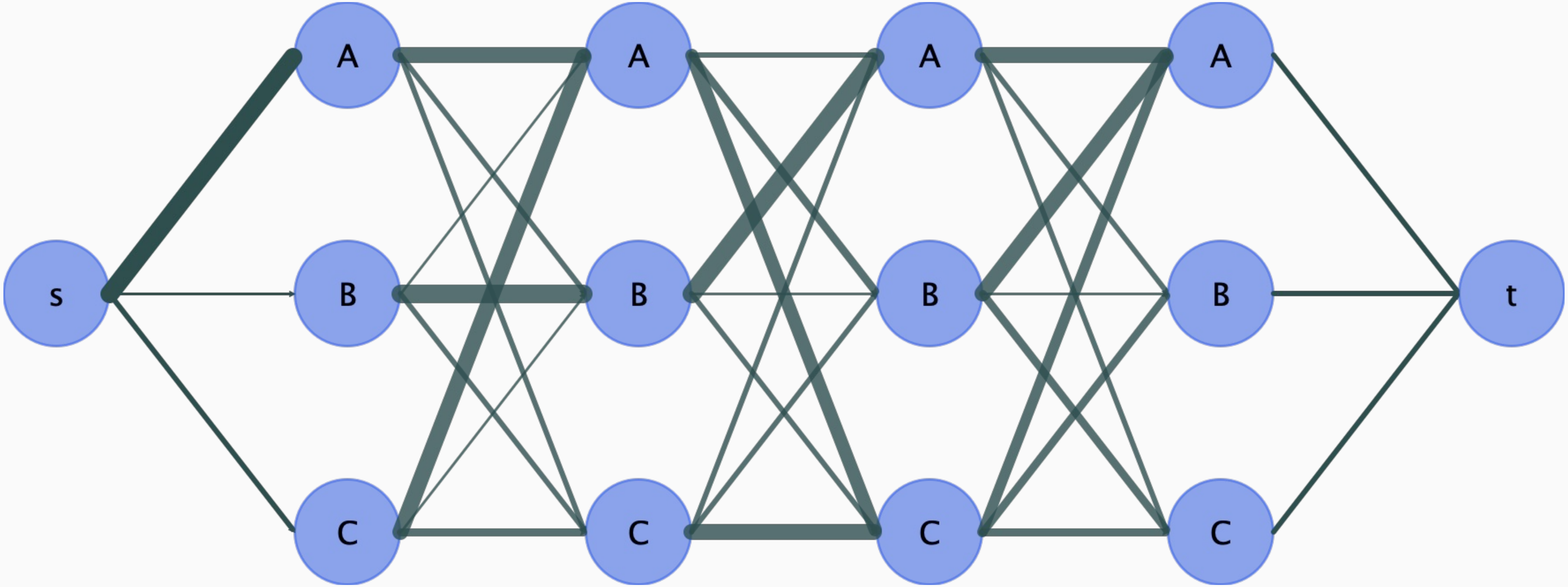
- At each state, choose the highest scoring next transition
  - Keep only one state in memory: The current state

- What is the problem?
  - Local decisions may override global optimum
  - Does not explore full search space

- Greedy algorithms can give the true optimum for special classes of problems
  - Eg: Maximum-spanning tree algorithms are greedy

Questions?

What would greedy search do on this graph?



Beam search

- Keep size-limited priority queue of states
  - Called the beam, sorted by probability for the state
- At each step:
  - Explore all transitions from the current state
  - Add all to beam and trim the size

What we might really want to do is to explore the full search space.

We cannot. Beam search is a compromise

Beam search: A compromise

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Example: Suppose we have a beam of size k = 2

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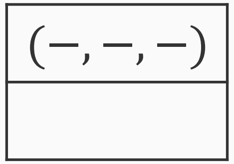

At the beginning, the beam has
only one element, the start state

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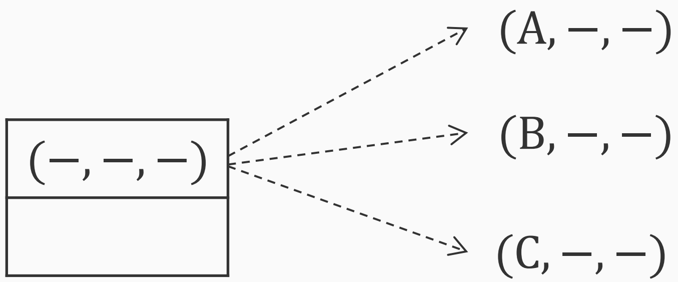

Expand all the states in the beam

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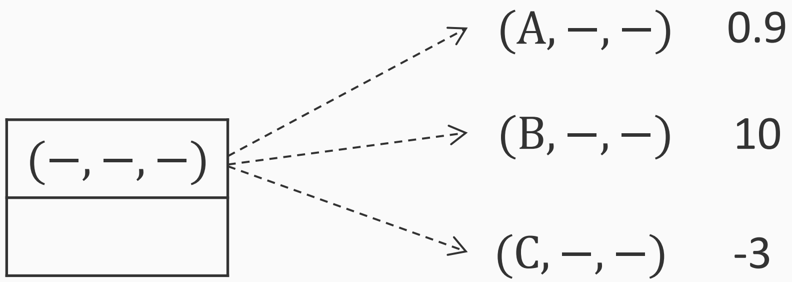

$(-,-,-)$

$(A,-,-)$ 0.9

$(B,-,-)$ 10

$(C,-,-)$ -3

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Score the newly created states

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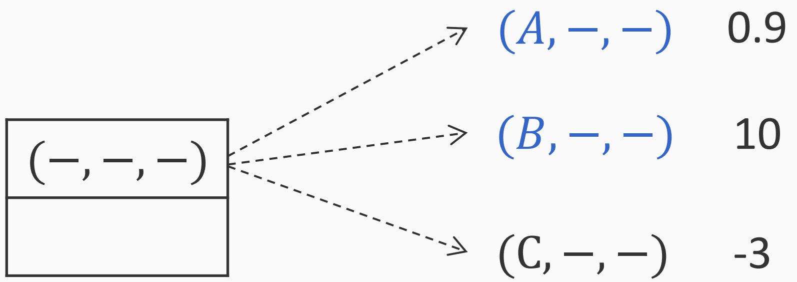
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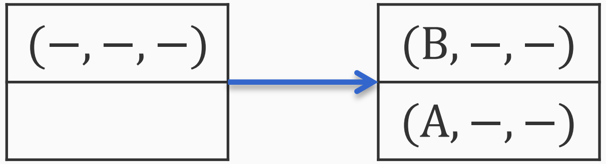

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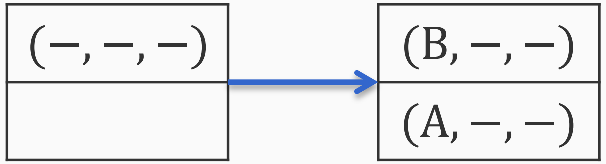

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Now we are ready for the next step

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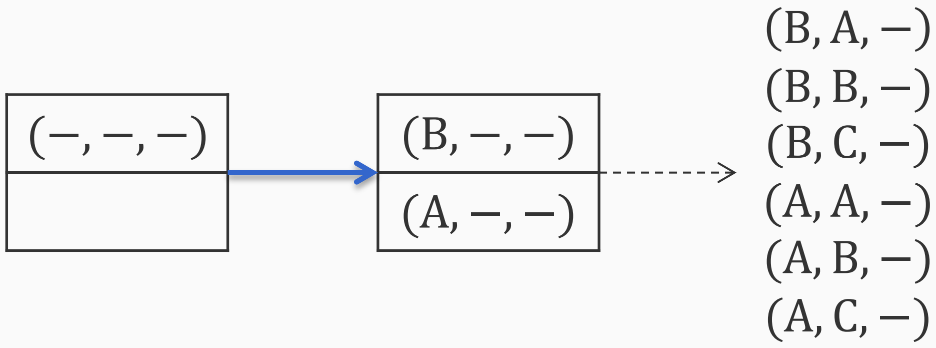

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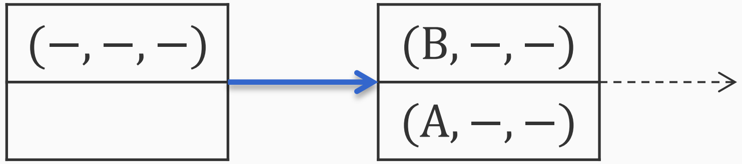

$(-,-,-)$

$(\mathrm{B},-,-)$

$(\mathrm{A},-,-)$

$(\mathrm{B},\mathrm{A},-)$	0.1
$(\mathrm{B},\mathrm{B},-)$	-3
$(\mathrm{B},\mathrm{C},-)$	10
$(\mathrm{A},\mathrm{A},-)$	20
$(\mathrm{A},\mathrm{B},-)$	-1
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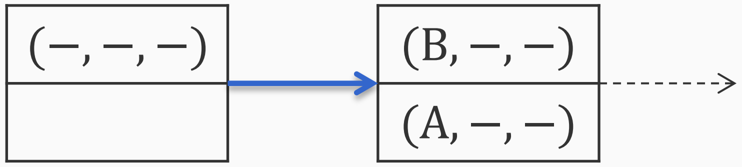

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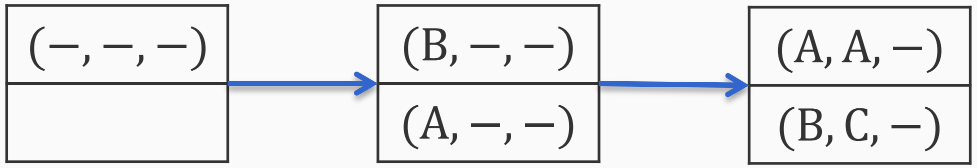

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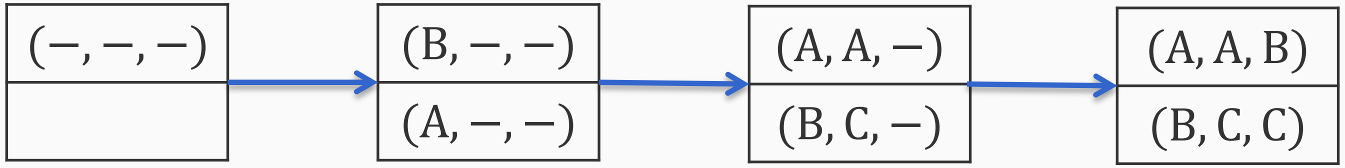

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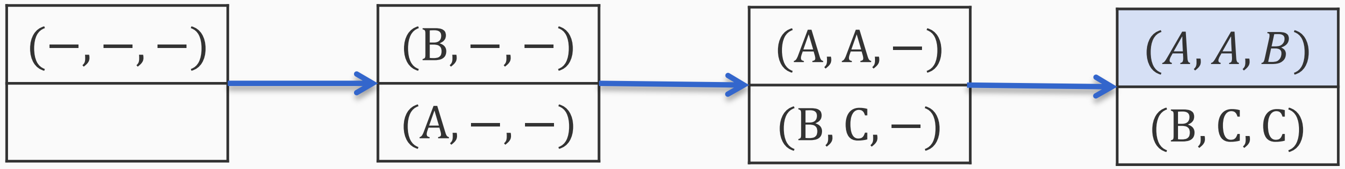

Final answer: Top of the beam at the end of search

Beam Search

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Pros

- Explores more than greedy search. Greedy search is beam search with beam size 1
- In general, easy to implement, very popular
- We get a set of sequences that we can then re-order or use in other ways

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- We get a set of sequences that we can then re-order or use in other ways

Cons

- A good state might fall out of the beam
- Can be still repetitive. Possible solution: add an n-gram penalty to penalize n-grams that get repeated
- Generated text may be *boring* for a reader

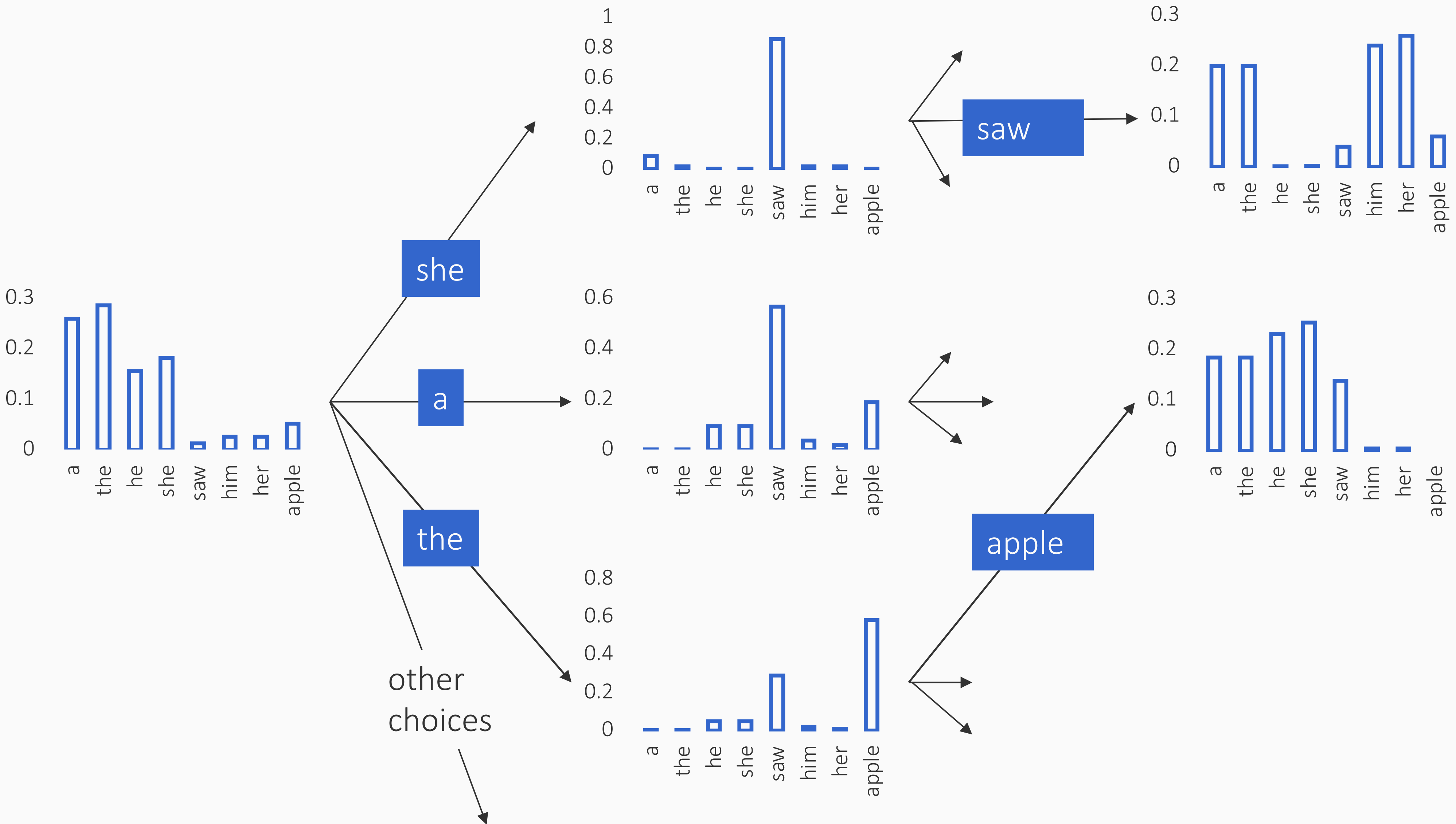
  Do we always choose the most probable next words? What makes a sequences of words interesting?

Sampling based approaches

Rather than picking the most probable next token, randomly pick one using the next token distribution

$$w_n \sim P\left(v \mid w_0 w_1 \cdots w_{\{n-1\}} \right)$$

Random sampling in our toy setting



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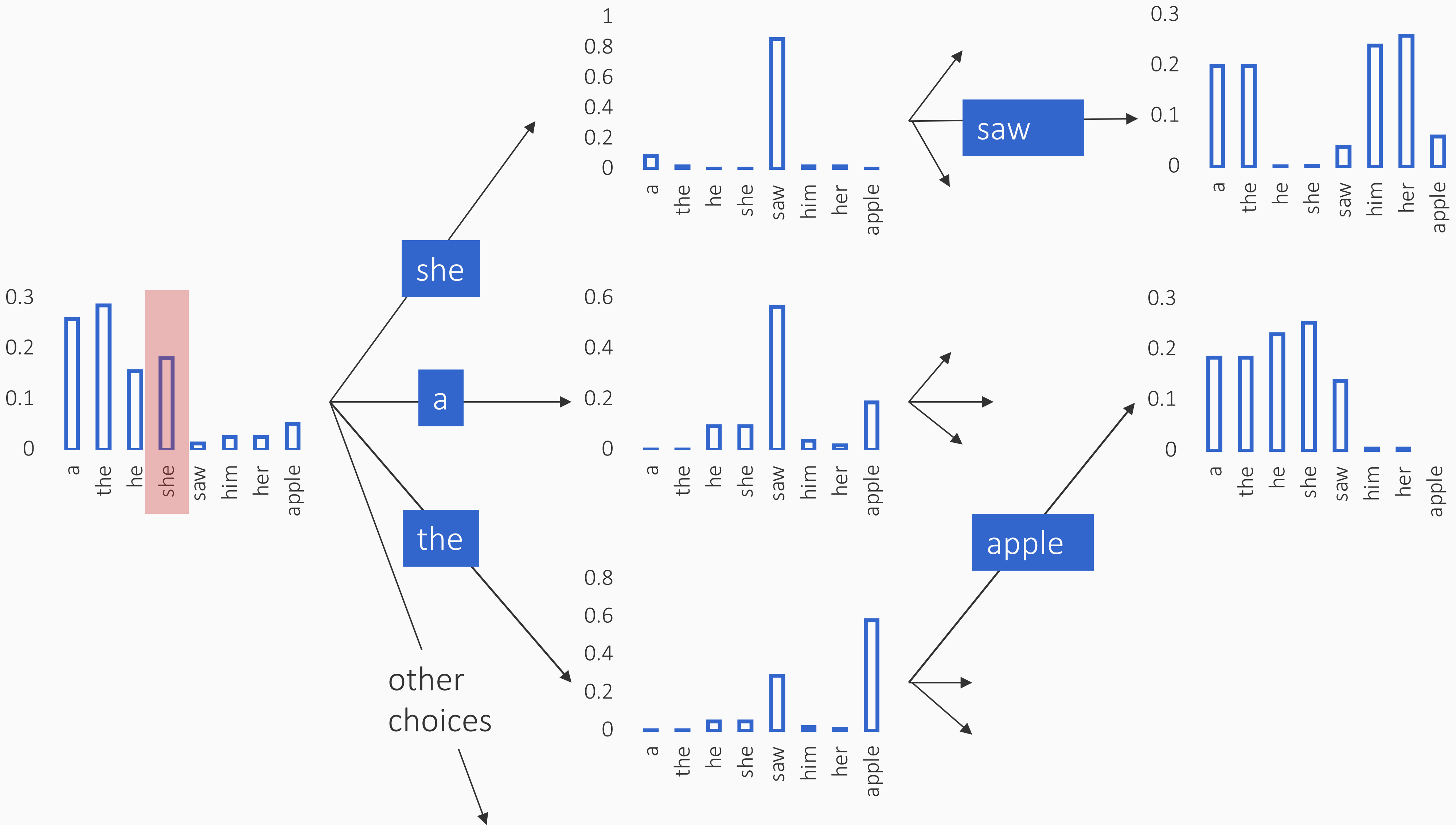

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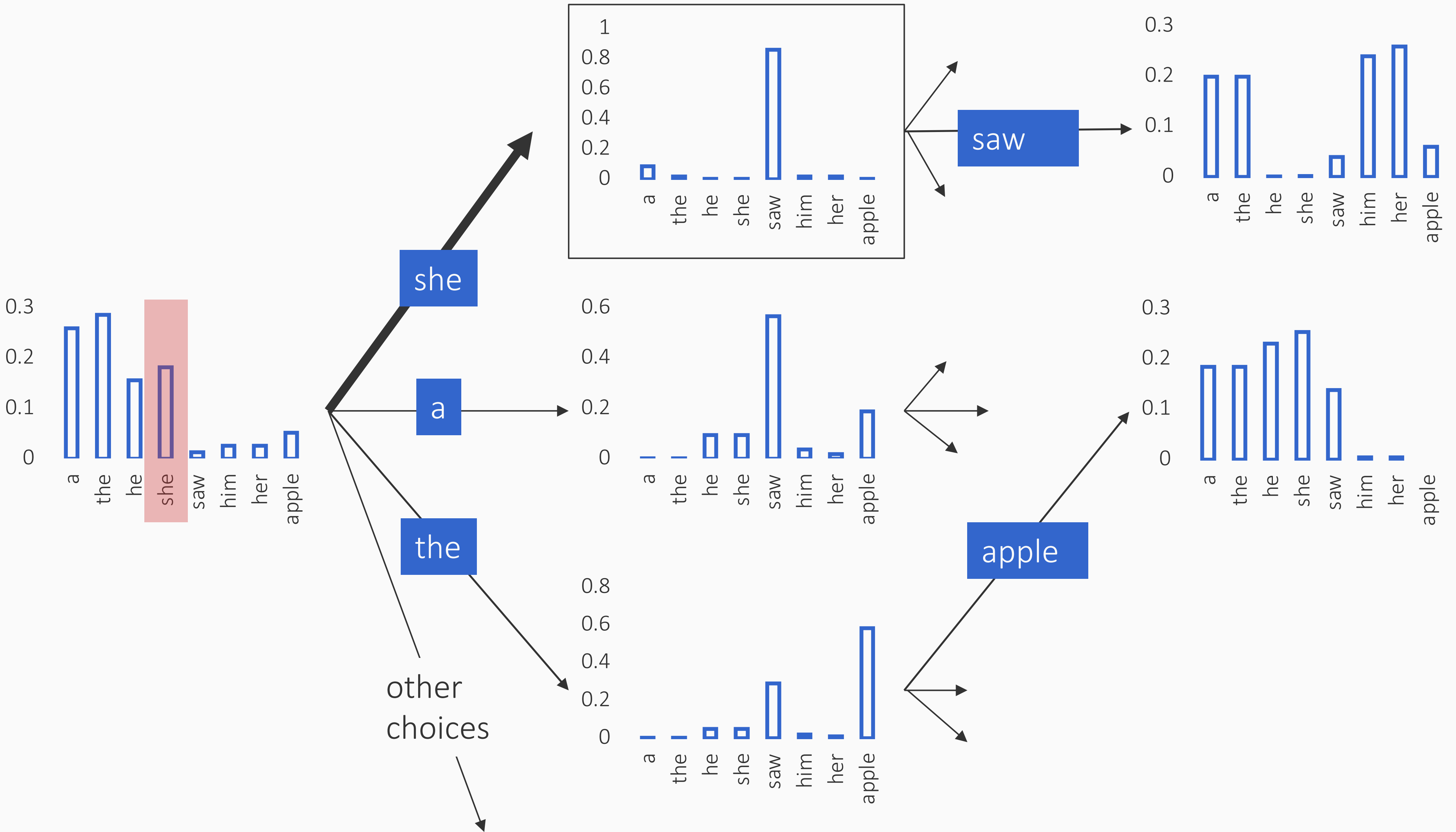

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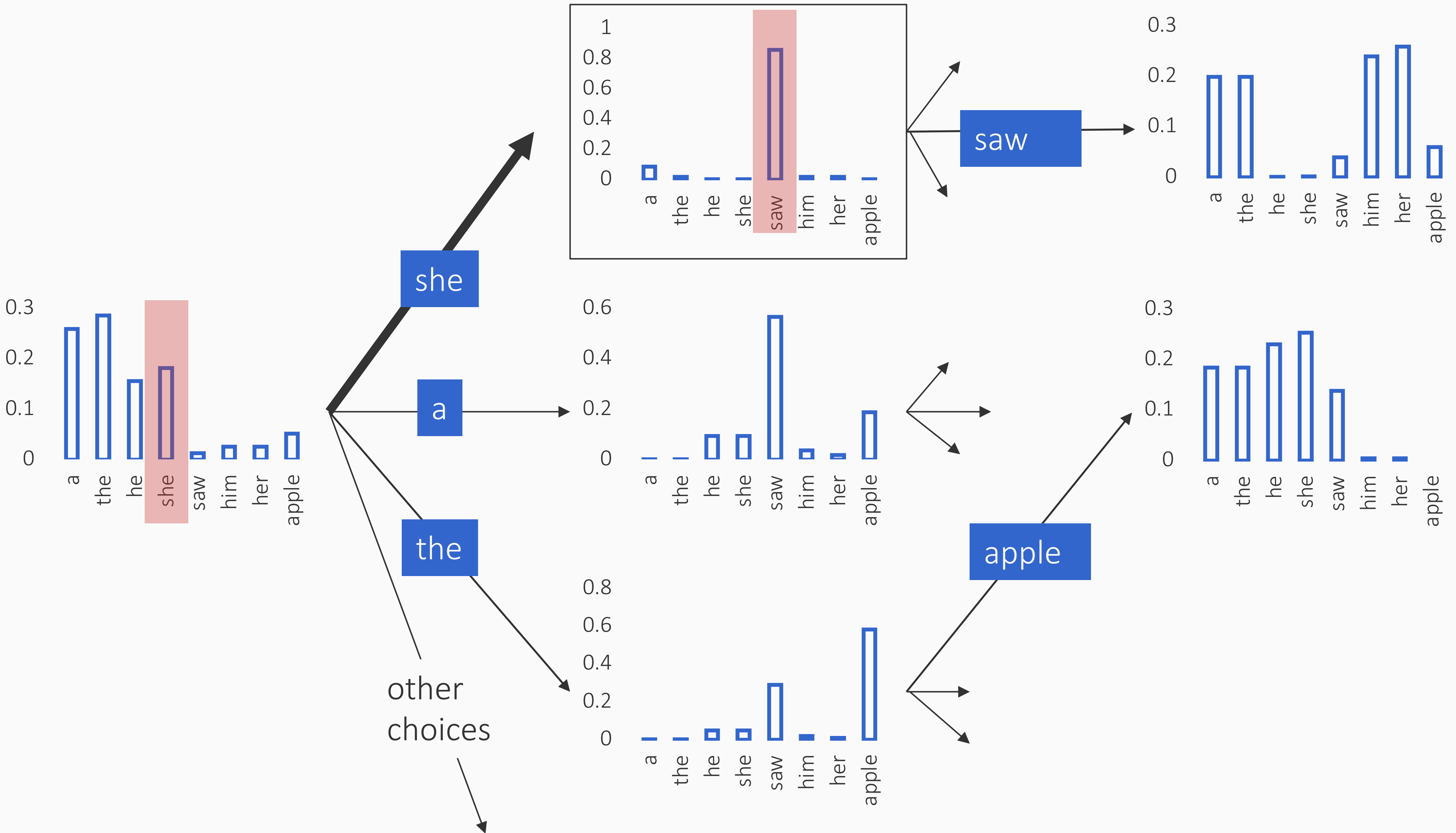

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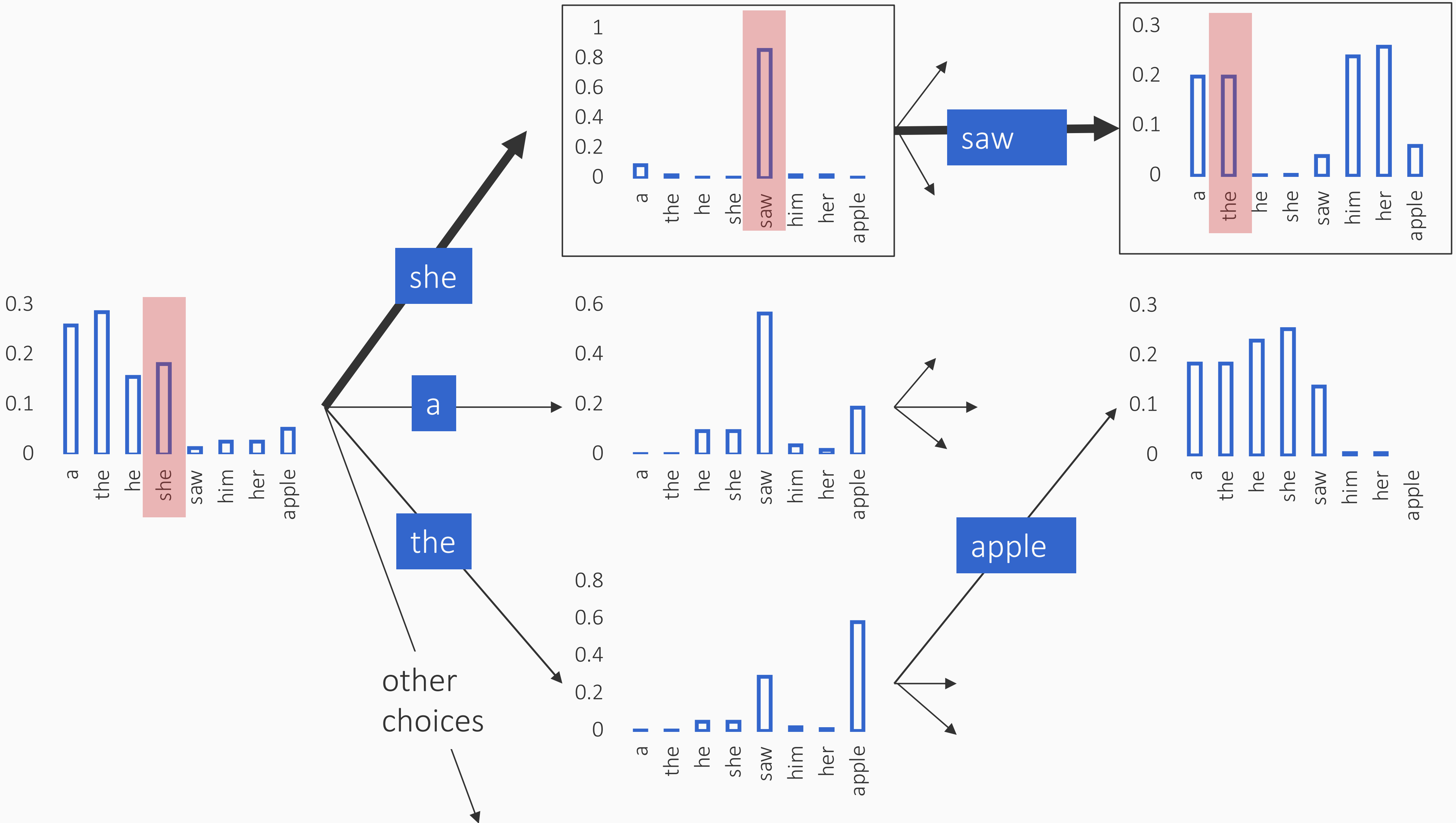

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$$w_n \sim P\left(v \mid w_0 w_1 \cdots w_{\{n-1\}} \right)$$

Pros

- Produces more interesting text
- Diverse outputs

Cons

- Does not produce coherent outputs. Why?

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$$P(token_i|context) = \frac{\exp\left(\frac{s_i}{T}\right)}{\sum_j \exp\left(\frac{s_j}{T}\right)}$$

When T is lower than 1, probabilities get more sharp and lower probabilities get diminished

When T = 0, all the probability is placed on the token with the highest s_i → Greedy decoding

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- Does not produce coherent outputs. Why?
  A solution: Use a *temperature* term in the softmax to make the probabilities “peaky”

Summary: Inference as graph search

- Inference with discrete random variables involves finding a score maximizing assignment to variables

- We can incrementally construct such an assignment using graph algorithms
  - Many inference algorithms are efficient dynamic programming formulations
  - General graph search is also helpful

- Popular heuristics in this family of methods:
  - Greedy search
  - Beam search
  - Random sampling and its variants