

# Probabilistic (Graphical) Models

## and inference

Oliver Obst · Autumn 2024



# Probabilistic (Graphical) Models and Inference

(PGM: Probabilistic Graphical Models: Principles and Techniques by Daphne Koller and Nir Friedman. MIT Press)

(PMLI: Probabilistic Machine Learning: An introduction by Kevin Murphy. MIT Press)

Week	Lecture	Required reading	Assessment
1 Monday, 4 March 2024	Introduction, Probability Theory	PGM Chapter 2, PMLI Chapter 6.1	
2 Monday, 11 March 2024	Directed and undirected networks introduction	PGM Chapter 3 & 4	Quiz 1
3 Monday, 18 March 2024	Variable elimination	PGM Chapter 9	
4 Monday, 25 March 2024	Belief propagation	PGM Chapter 10/11	Quiz 2
5 Monday, 1 April 2024	public holiday		5 April 2024: census date
6 Monday, 8 April 2024	Message passing / Graph neural networks	<a href="https://distill.pub/2021/gnn-intro/">https://distill.pub/2021/gnn-intro/</a>	
7 Monday, 15 April 2024	Sampling		Quiz 3
8 Monday, 22 April 2024	Mid-term break		
9 Monday, 29 April 2024	Variational inference		Intra-session exam
10 Monday, 6 May 2024	Autoregressive models		Quiz 4
11 Monday, 13 May 2024	Variational Auto-Encoders		
12 Monday, 20 May 2024	GANs		Quiz 5
13 Monday, 27 May 2024	Energy-based models		
14 Monday, 3 June 2024	Evaluating generative models		Quiz 6
Monday, 17 June 2024			Project due

# Conditional probability queries

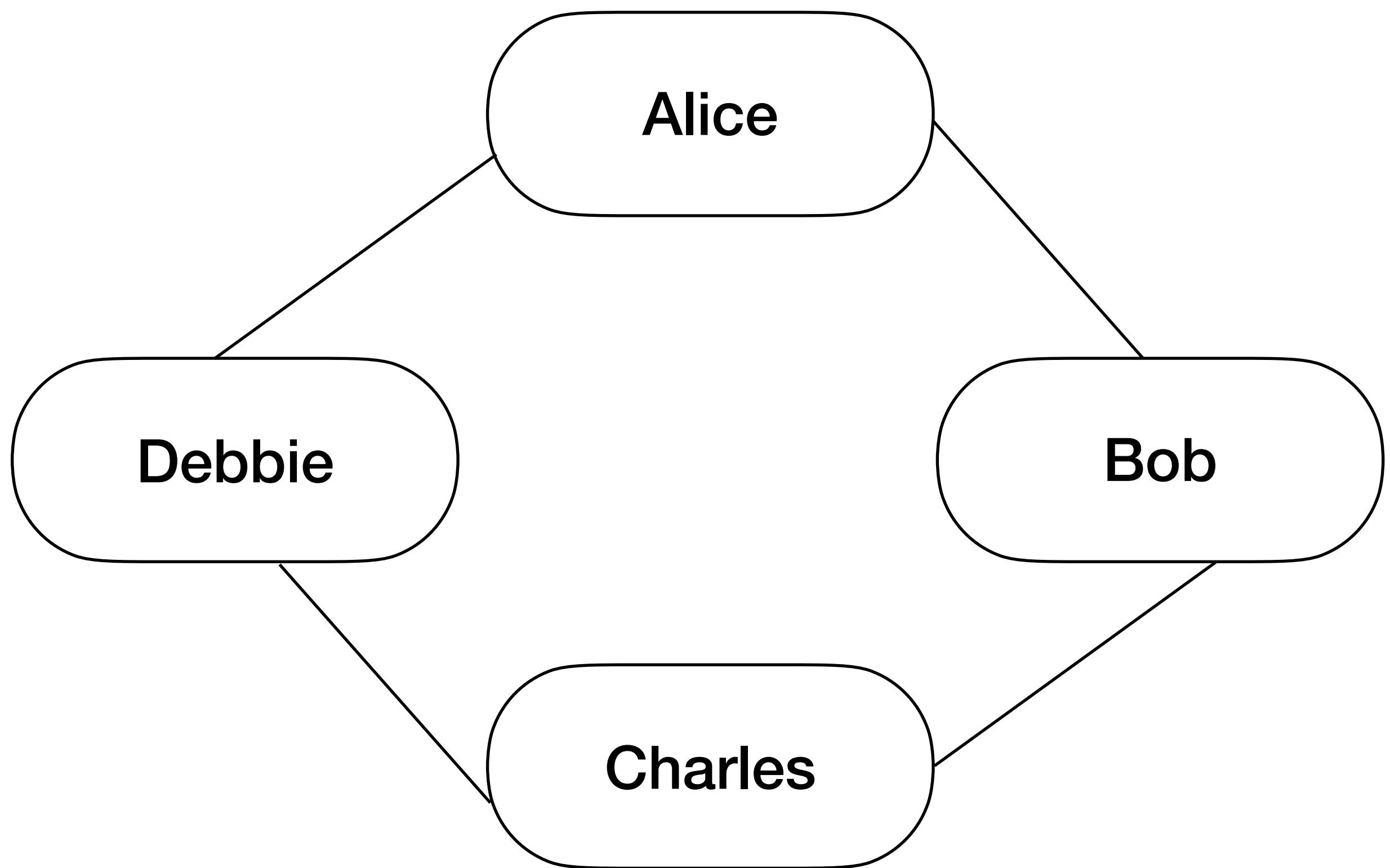
- Evidence:  $E = e$
- Query: a subset of variables  $Y$
- Task: compute  $P(Y | E = e)$

# Message passing algorithms

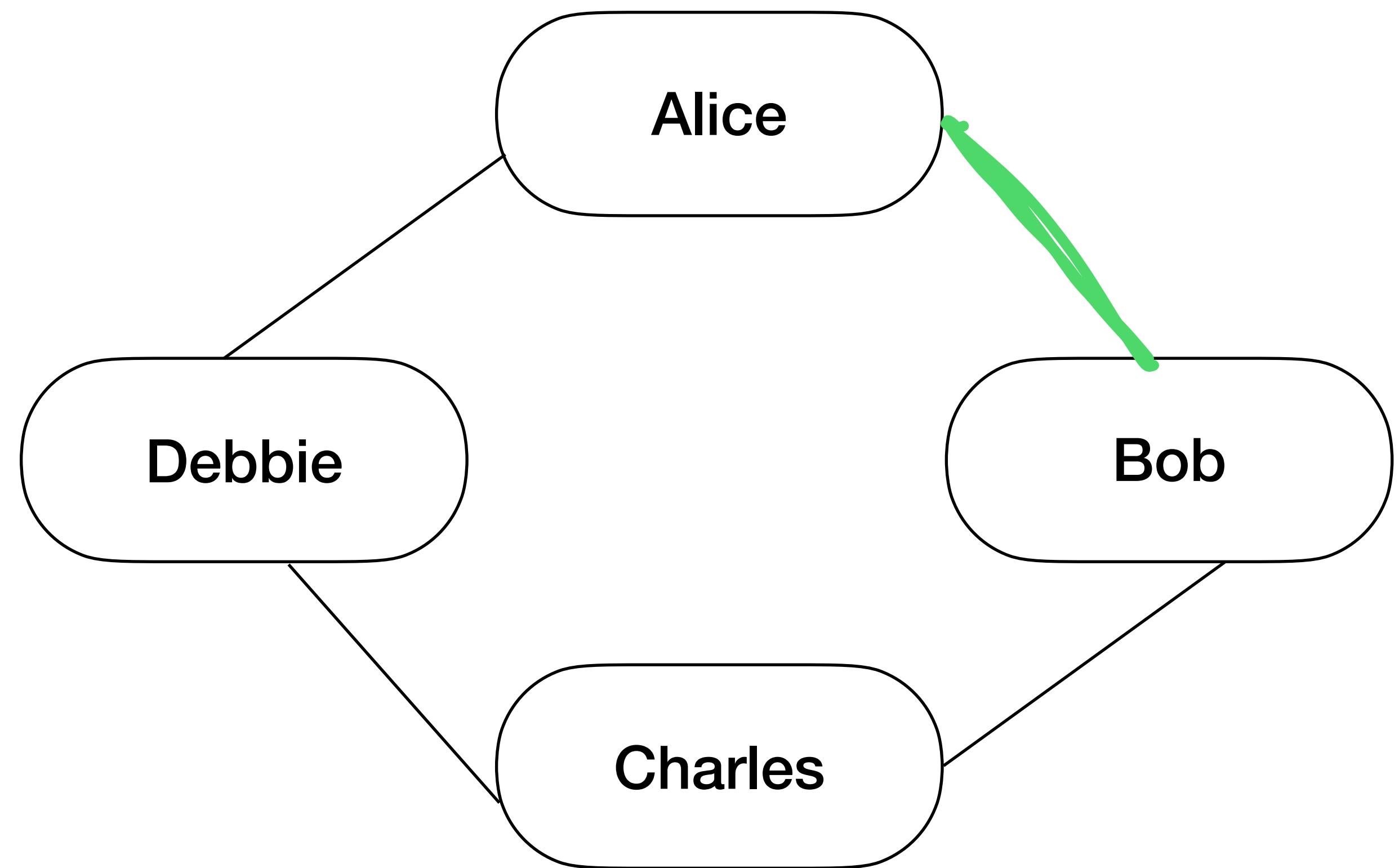
- We continue to do inference on graphical models
- But instead of Variable Elimination (last week), we use “Message Passing”

# Markov Networks

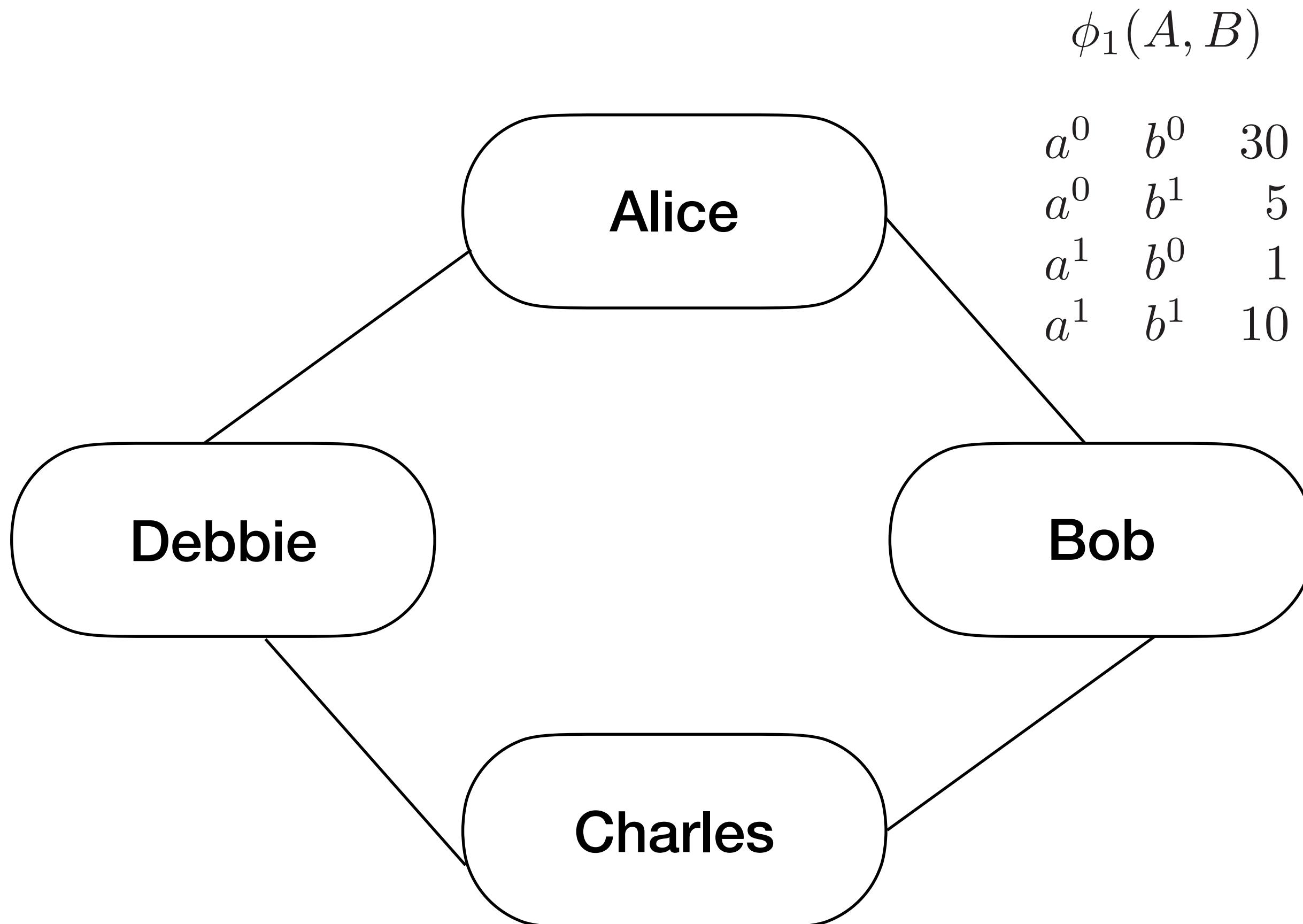
# Pairwise Markov Networks



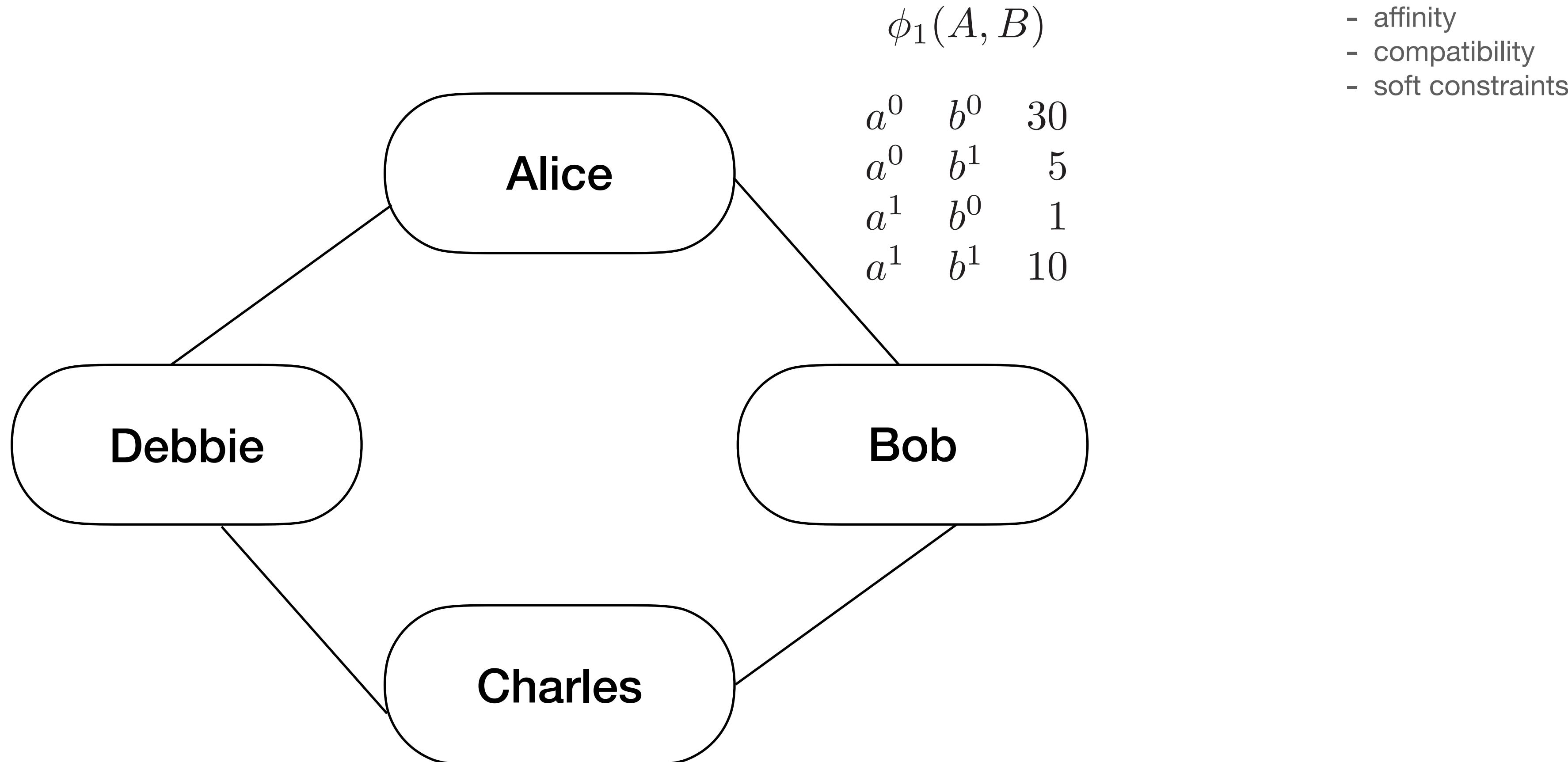
# Pairwise Markov Networks



# Pairwise Markov Networks

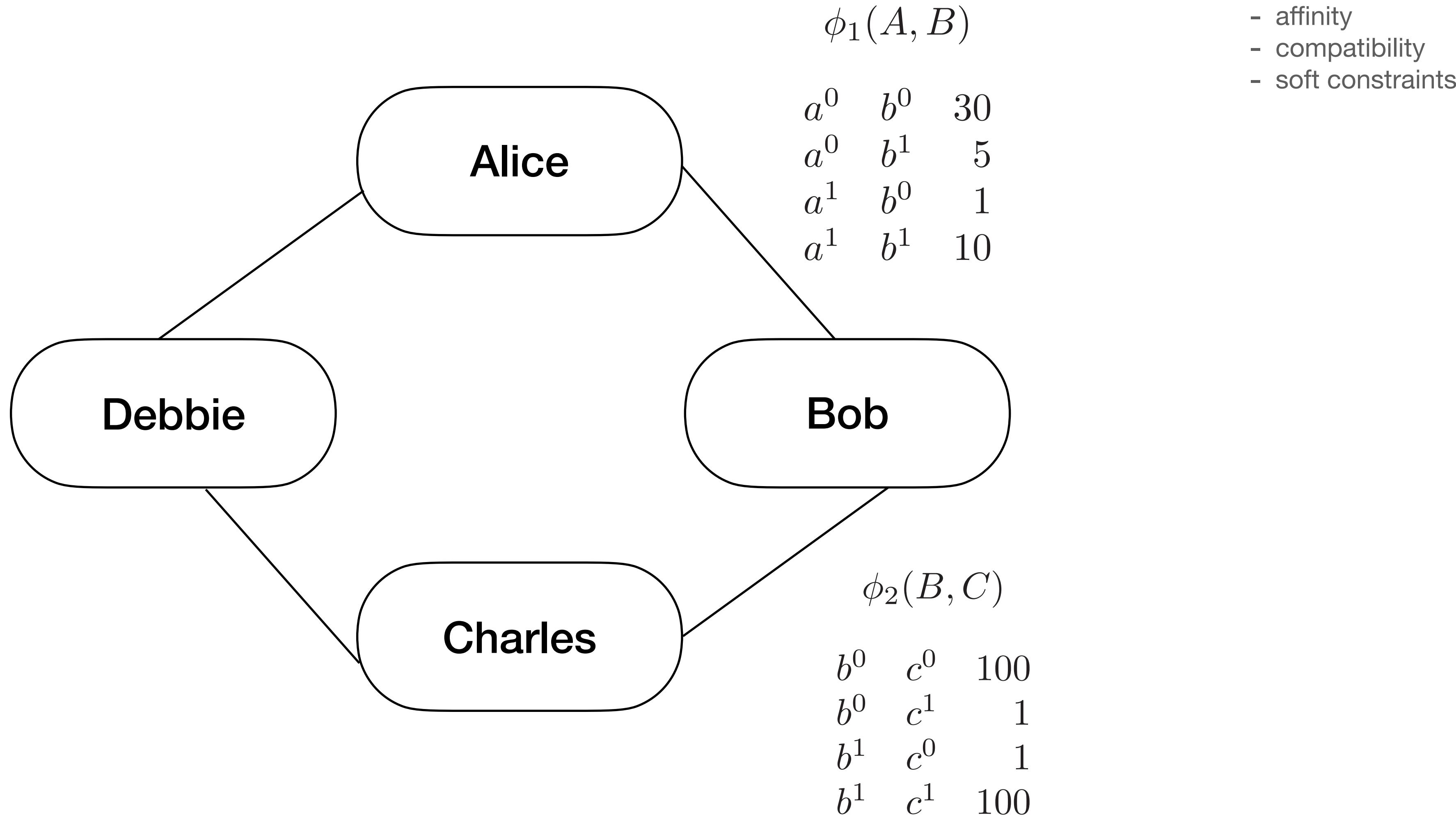


# Pairwise Markov Networks



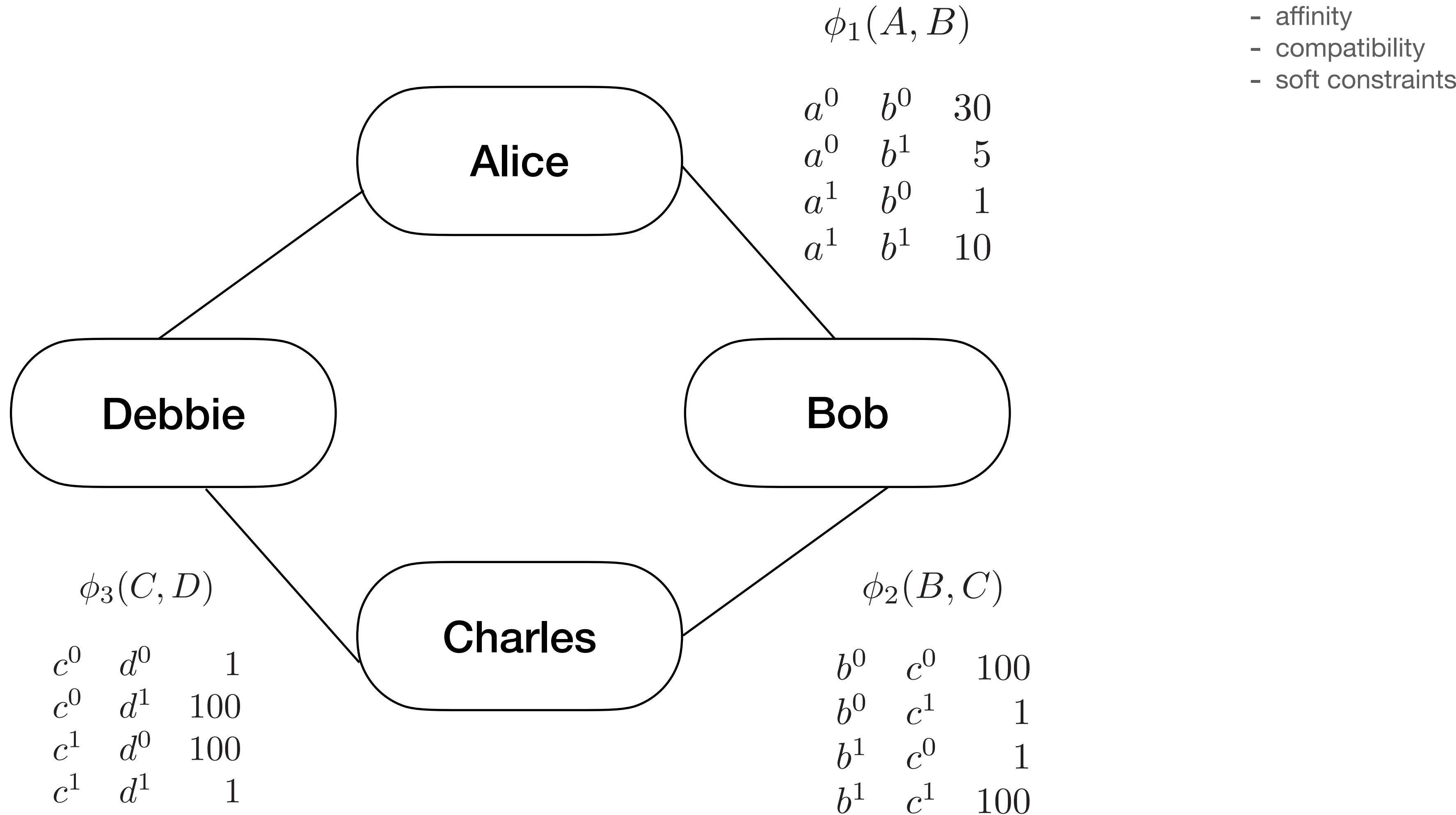
- affinity
- compatibility
- soft constraints

# Pairwise Markov Networks



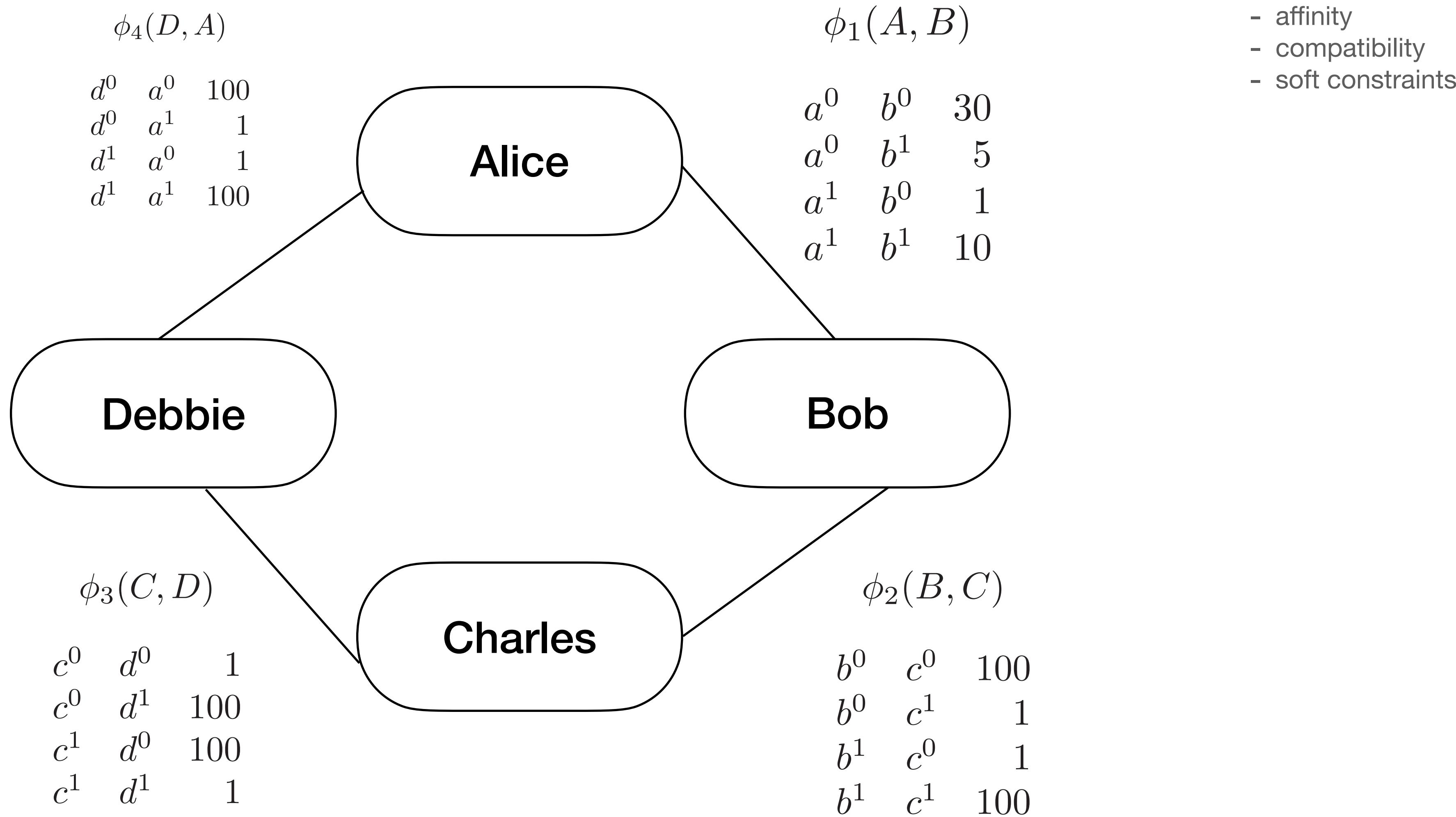
- affinity
- compatibility
- soft constraints

# Pairwise Markov Networks



- affinity
- compatibility
- soft constraints

# Pairwise Markov Networks



- affinity
- compatibility
- soft constraints

$$\tilde{P}(A, B, C, D) = \phi_1(A, B) \times \phi_2(B, C) \times \phi_3(C, D) \times \phi_4(D, A)$$

Unnormalised measure

$\phi_4(D, A)$	$\phi_1(A, B)$
$d^0 \quad a^0 \quad 100$	$a^0 \quad b^0 \quad 30$
$d^0 \quad a^1 \quad 1$	$a^0 \quad b^1 \quad 5$
$d^1 \quad a^0 \quad 1$	$a^1 \quad b^0 \quad 1$
$d^1 \quad a^1 \quad 100$	$a^1 \quad b^1 \quad 10$

$\phi_4(D, A)$	$\phi_1(A, B)$	$\phi_2(B, C)$
$d^0 \quad d^0 \quad 1$	$b^0 \quad c^0 \quad 100$	
$d^0 \quad d^1 \quad 100$	$b^0 \quad c^1 \quad 1$	
$d^1 \quad d^0 \quad 100$	$b^1 \quad c^0 \quad 1$	
$d^1 \quad d^1 \quad 1$	$b^1 \quad c^1 \quad 100$	

$$\tilde{P}(A, B, C, D) = \phi_1(A, B) \times \phi_2(B, C) \times \phi_3(C, D) \times \phi_4(D, A)$$

Unnormalised measure

$$P(A, B, C, D) = \frac{1}{Z} \tilde{P}(A, B, C, D)$$

Partition function

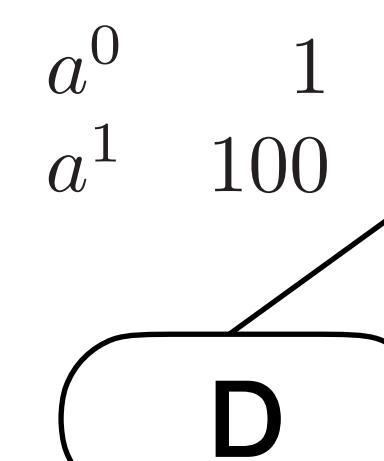
Assignment				Unnormalized
$a^0$	$b^0$	$c^0$	$d^0$	300,000
$a^0$	$b^0$	$c^0$	$d^1$	300,000
$a^0$	$b^0$	$c^1$	$d^0$	300,000
$a^0$	$b^0$	$c^1$	$d^1$	30
$a^0$	$b^1$	$c^0$	$d^0$	500
$a^0$	$b^1$	$c^0$	$d^1$	500
$a^0$	$b^1$	$c^1$	$d^0$	5,000,000
$a^0$	$b^1$	$c^1$	$d^1$	500
$a^1$	$b^0$	$c^0$	$d^0$	100
$a^1$	$b^0$	$c^0$	$d^1$	1,000,000
$a^1$	$b^0$	$c^1$	$d^0$	100
$a^1$	$b^0$	$c^1$	$d^1$	100
$a^1$	$b^1$	$c^0$	$d^0$	10
$a^1$	$b^1$	$c^0$	$d^1$	100,000
$a^1$	$b^1$	$c^1$	$d^0$	100,000
$a^1$	$b^1$	$c^1$	$d^1$	100,000

$\phi_4(D, A)$

$\phi_1(A, B)$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$a^0$	$b^0$	30
$a^0$	$b^1$	5
$a^1$	$b^0$	1
$a^1$	$b^1$	10



$\phi_3(C, D)$

$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$b^0$	$c^0$	100
$b^0$	$c^1$	1
$b^1$	$c^0$	1
$b^1$	$c^1$	100

$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$b^1$	$c^1$	100
-------	-------	-----

$$\tilde{P}(A, B, C, D) = \phi_1(A, B) \times \phi_2(B, C) \times \phi_3(C, D) \times \phi_4(D, A)$$

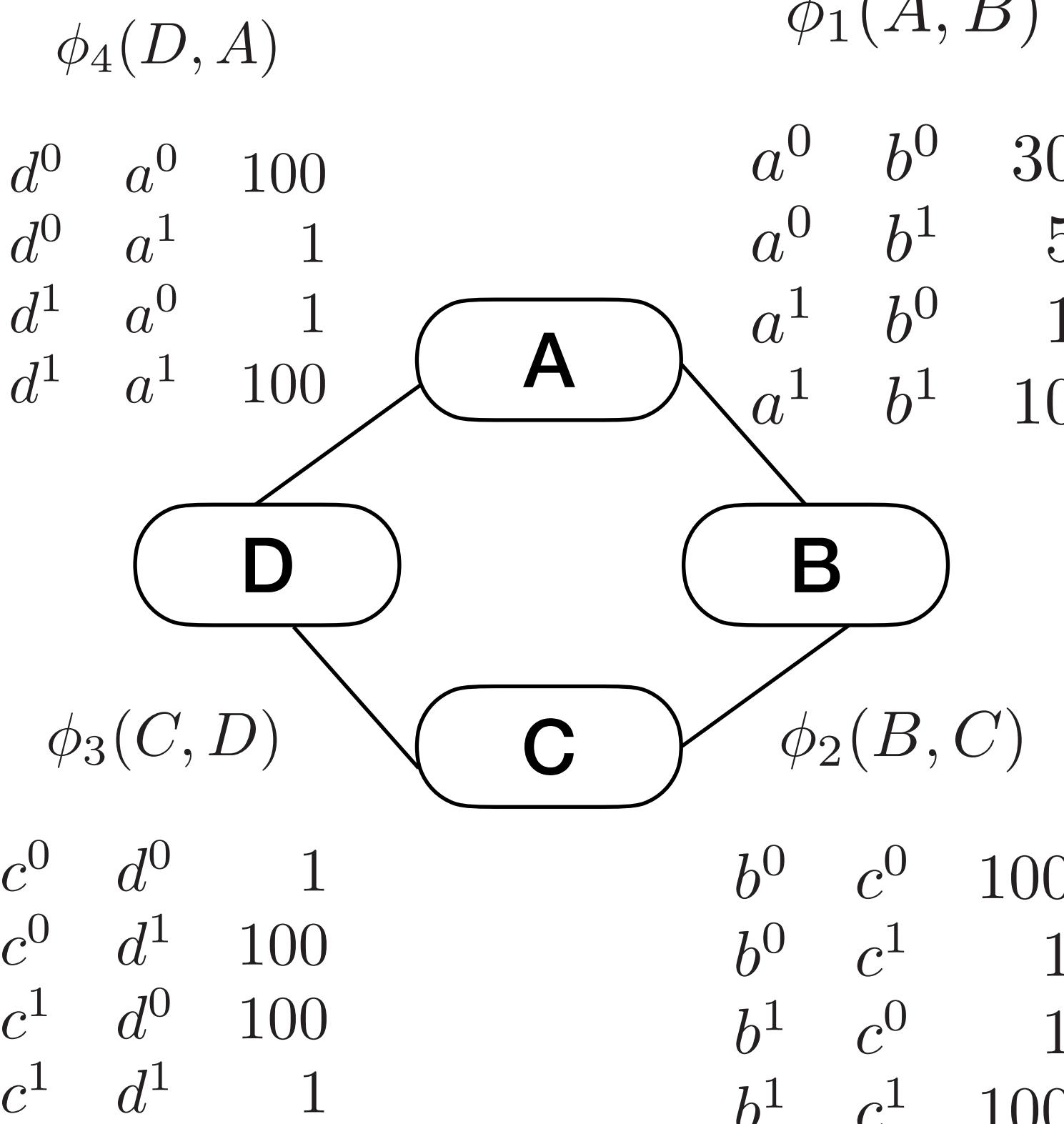
Unnormalised measure

$$P(A, B, C, D) = \frac{1}{Z} \tilde{P}(A, B, C, D)$$

Partition function

Assignment				Unnormalized	Normalized
$a^0$	$b^0$	$c^0$	$d^0$	300,000	0.04
$a^0$	$b^0$	$c^0$	$d^1$	300,000	0.04
$a^0$	$b^0$	$c^1$	$d^0$	300,000	0.04
$a^0$	$b^0$	$c^1$	$d^1$	30	$4.1 \cdot 10^{-6}$
$a^0$	$b^1$	$c^0$	$d^0$	500	$6.9 \cdot 10^{-5}$
$a^0$	$b^1$	$c^0$	$d^1$	500	$6.9 \cdot 10^{-5}$
$a^0$	$b^1$	$c^1$	$d^0$	5,000,000	0.69
$a^0$	$b^1$	$c^1$	$d^1$	500	$6.9 \cdot 10^{-5}$
$a^1$	$b^0$	$c^0$	$d^0$	100	$1.4 \cdot 10^{-5}$
$a^1$	$b^0$	$c^0$	$d^1$	1,000,000	0.14
$a^1$	$b^0$	$c^1$	$d^0$	100	$1.4 \cdot 10^{-5}$
$a^1$	$b^0$	$c^1$	$d^1$	100	$1.4 \cdot 10^{-5}$
$a^1$	$b^1$	$c^0$	$d^0$	10	$1.4 \cdot 10^{-6}$
$a^1$	$b^1$	$c^0$	$d^1$	100,000	0.014
$a^1$	$b^1$	$c^1$	$d^0$	100,000	0.014
$a^1$	$b^1$	$c^1$	$d^1$	100,000	0.014

$\underline{Z}$



What does the pairwise factor  $\phi_1(A, B)$  mean?

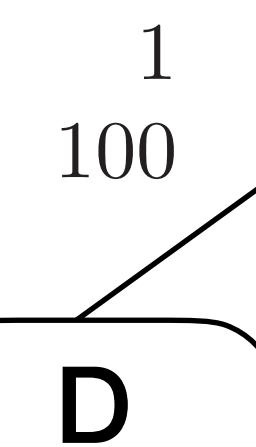
It is the local “happiness” between A and B. How does it relate to a probability distribution?

$$\phi_4(D, A)$$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$$\phi_1(A, B)$$

$a^0$	$b^0$	30
$a^0$	$b^1$	5
$a^1$	$b^0$	1
$a^1$	$b^1$	10



$$\phi_3(C, D)$$

$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$$\phi_2(B, C)$$

$b^0$	$c^0$	100
$b^0$	$c^1$	1
$b^1$	$c^0$	1
$b^1$	$c^1$	100

What does the pairwise factor  $\phi_1(A, B)$  mean?

It is the local “happiness” between A and B. How does it relate to a probability distribution?

- $P(A, B)$
- $P(A | B)$
- $P(A, B | C, D)$
- ?

$\phi_4(D, A)$	$a^0$	$b^0$	30
$d^0$	$a^0$	100	
$d^0$	$a^1$	1	
$d^1$	$a^0$	1	
$d^1$	$a^1$	100	
	$a^1$	$b^0$	1
	$a^1$	$b^1$	10
$\phi_3(C, D)$	$b^0$	$c^0$	100
$c^0$	$d^0$	1	
$c^0$	$d^1$	100	
$c^1$	$d^0$	100	
$c^1$	$d^1$	1	
	$b^1$	$c^1$	100

```

graph TD
    A((A)) -- "phi_1(A, B)" --> B((B))
    A -- "phi_1(A, D)" --> D((D))
    D -- "phi_3(C, D)" --> C((C))
    D -- "phi_2(B, C)" --> B
    C -- "phi_2(B, C)" --> B
  
```

What does the pairwise factor  $\phi_1(A, B)$  mean?

$$P_{\phi}(A, B)$$

$a^0$	$b^0$	0.13
$a^0$	$b^1$	0.69
$a^1$	$b^0$	0.14
$a^1$	$b^1$	0.04

$$\phi = \{\phi_1, \phi_2, \phi_3, \phi_4\}$$

$$\phi_4(D, A)$$

$$\phi_1(A, B)$$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$$a^0 \quad b^0 \quad 30$$

$$a^0 \quad b^1 \quad 5$$

$$a^1 \quad b^0 \quad 1$$

$$a^1 \quad b^1 \quad 10$$

**D**

**B**

**C**



$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$$b^0 \quad c^0 \quad 100$$

$$b^0 \quad c^1 \quad 1$$

$$b^1 \quad c^0 \quad 1$$

$$b^1 \quad c^1 \quad 100$$

What does the pairwise factor  $\phi_1(A, B)$  mean?

$$P_{\phi}(A, B)$$

$a^0$	$b^0$	0.13
$a^0$	$b^1$	0.69
$a^1$	$b^0$	0.14
$a^1$	$b^1$	0.04

$$\phi = \{\phi_1, \phi_2, \phi_3, \phi_4\}$$

$$\phi_4(D, A)$$

$$\phi_1(A, B)$$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$$a^0 \quad b^0 \quad 30$$

$$a^0 \quad b^1 \quad 5$$

$$a^1 \quad b^0 \quad 1$$

$$a^1 \quad b^1 \quad 10$$

**D**

**B**

**C**



$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$$b^0 \quad c^0 \quad 100$$

$$b^0 \quad c^1 \quad 1$$

$$b^1 \quad c^0 \quad 1$$

$$b^1 \quad c^1 \quad 100$$

What does the pairwise factor  $\phi_1(A, B)$  mean?

$$P_{\phi}(A, B)$$

$a^0$	$b^0$	0.13
$a^0$	$b^1$	0.69
$a^1$	$b^0$	0.14
$a^1$	$b^1$	0.04

$$\phi = \{\phi_1, \phi_2, \phi_3, \phi_4\}$$

$$\phi_4(D, A)$$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$$\phi_1(A, B)$$

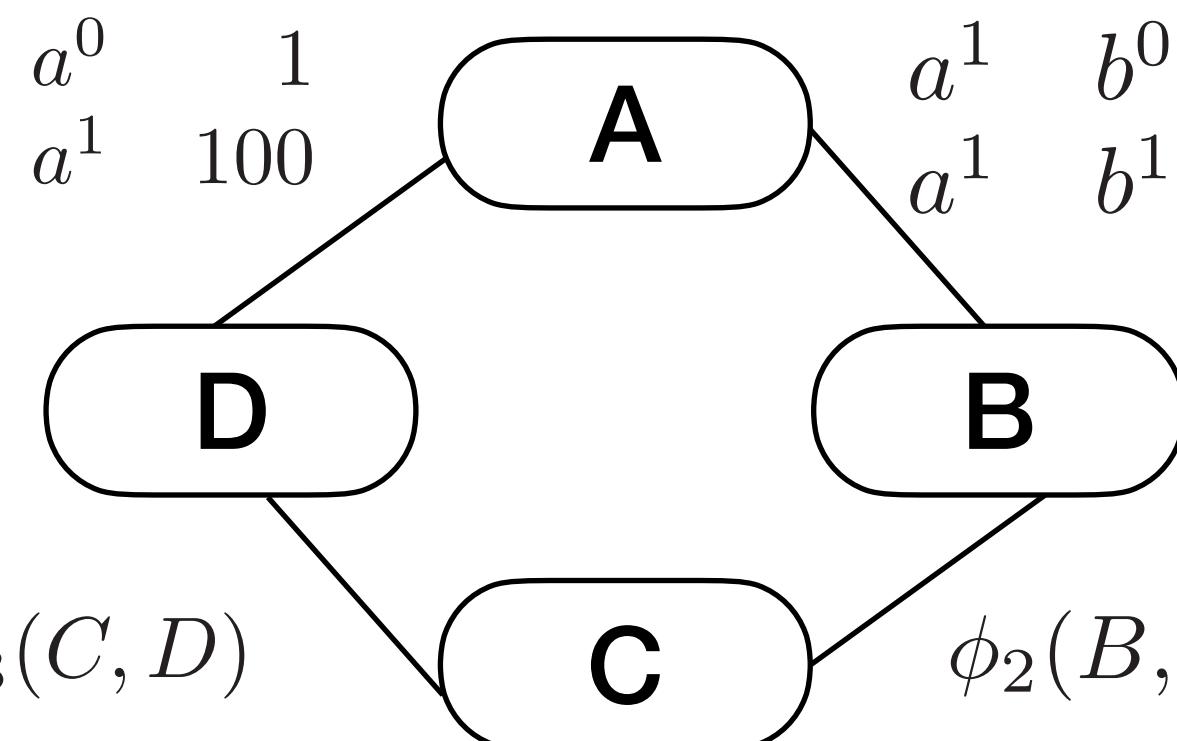
$a^0$	$b^0$	30
$a^0$	$b^1$	5
$a^1$	$b^0$	1
$a^1$	$b^1$	10

$$\phi_3(C, D)$$

$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$b^0$	$c^0$	100
$b^0$	$c^1$	1
$b^1$	$c^0$	1
$b^1$	$c^1$	100

$$\phi_2(B, C)$$



$$\phi_3(C, D)$$

$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$$\phi_4(D, A)$$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$a^0$	$b^0$	30
$a^0$	$b^1$	5
$a^1$	$b^0$	1
$a^1$	$b^1$	10

What does the pairwise factor  $\phi_1(A, B)$  mean?

$$P_{\phi}(A, B)$$

$$\phi = \{\phi_1, \phi_2, \phi_3, \phi_4\}$$

$a^0$	$b^0$	<u>0.13</u>
$a^0$	$b^1$	<u>0.69</u>
$a^1$	$b^0$	0.14
$a^1$	$b^1$	0.04

$$\phi_4(D, A)$$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$$\phi_1(A, B)$$

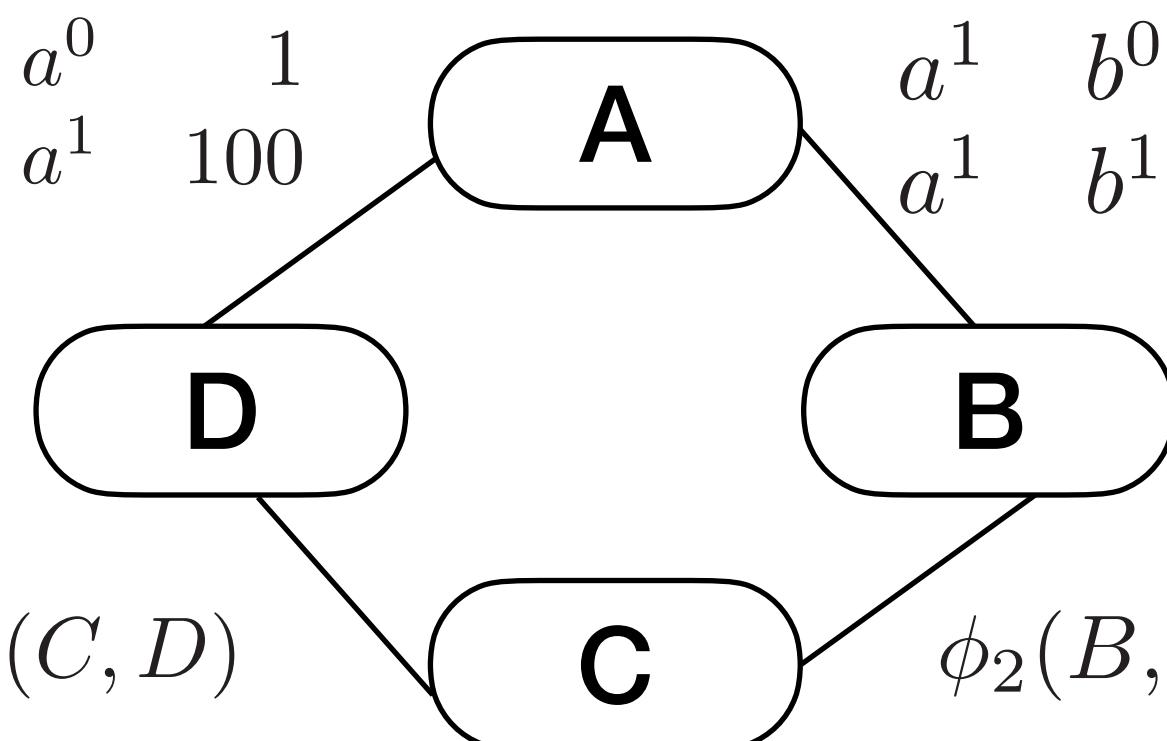
$a^0$	$b^0$	<u>30</u>
$a^0$	$b^1$	<u>5</u>
$a^1$	$b^0$	1
$a^1$	$b^1$	10

$$\phi_3(C, D)$$

$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$b^0$	$c^0$	100
$b^0$	$c^1$	1
$b^1$	$c^0$	1
$b^1$	$c^1$	100

$$\phi_2(B, C)$$



What does the pairwise factor  $\phi_1(A, B)$  mean?

$$P_{\phi}(A, B)$$

$$\phi = \{\phi_1, \phi_2, \phi_3, \phi_4\}$$

$a^0$	$b^0$	<u>0.13</u>
$a^0$	$b^1$	<u>0.69</u>
$a^1$	$b^0$	0.14
$a^1$	$b^1$	0.04

$$\phi_4(D, A)$$

$d^0$	$a^0$	100
$d^0$	$a^1$	1
$d^1$	$a^0$	1
$d^1$	$a^1$	100

$$\phi_1(A, B)$$

$a^0$	$b^0$	<u>30</u>
$a^0$	$b^1$	<u>5</u>
$a^1$	$b^0$	1
$a^1$	$b^1$	10

$$\phi_3(C, D)$$

$c^0$	$d^0$	1
$c^0$	$d^1$	100
$c^1$	$d^0$	100
$c^1$	$d^1$	1

$b^0$	$c^0$	100
$b^0$	$c^1$	1
$b^1$	$c^0$	1
$b^1$	$c^1$	100



What does the pairwise factor  $\phi_1(A, B)$  mean?

$$P_{\phi}(A, B)$$

$$\phi = \{\phi_1, \phi_2, \phi_3, \phi_4\}$$

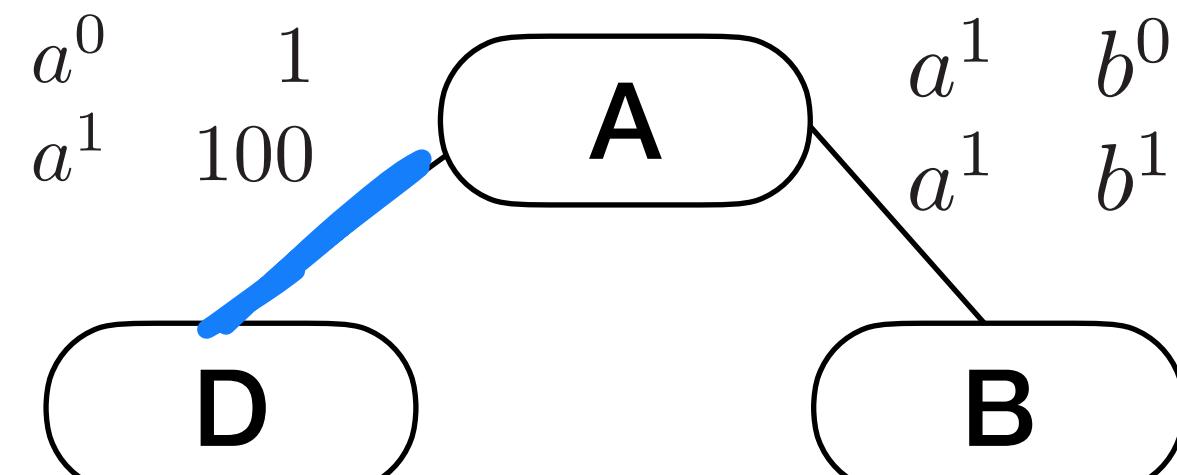
$a^0$	$b^0$	<u>0.13</u>
$a^0$	$b^1$	<u>0.69</u>
$a^1$	$b^0$	0.14
$a^1$	$b^1$	0.04

$$\phi_4(D, A)$$

$$\begin{array}{lll} d^0 & a^0 & 100 \\ d^0 & a^1 & 1 \\ d^1 & a^0 & 1 \\ d^1 & a^1 & 100 \end{array}$$

$$\phi_1(A, B)$$

$$\begin{array}{lll} a^0 & b^0 & 30 \\ a^0 & b^1 & 5 \\ a^1 & b^0 & 1 \\ a^1 & b^1 & 10 \end{array}$$



$$\phi_3(C, D)$$

$$\begin{array}{lll} c^0 & d^0 & 1 \\ c^0 & d^1 & 100 \\ c^1 & d^0 & 100 \\ c^1 & d^1 & 1 \end{array}$$

$$\begin{array}{lll} b^0 & c^0 & 100 \\ b^0 & c^1 & 1 \\ b^1 & c^0 & 1 \\ b^1 & c^1 & 100 \end{array}$$

$$\phi_2(B, C)$$

# Pairwise Markov Networks

- A pairwise Markov network is an undirected graph whose nodes are random variables  $X_1, \dots, X_n$

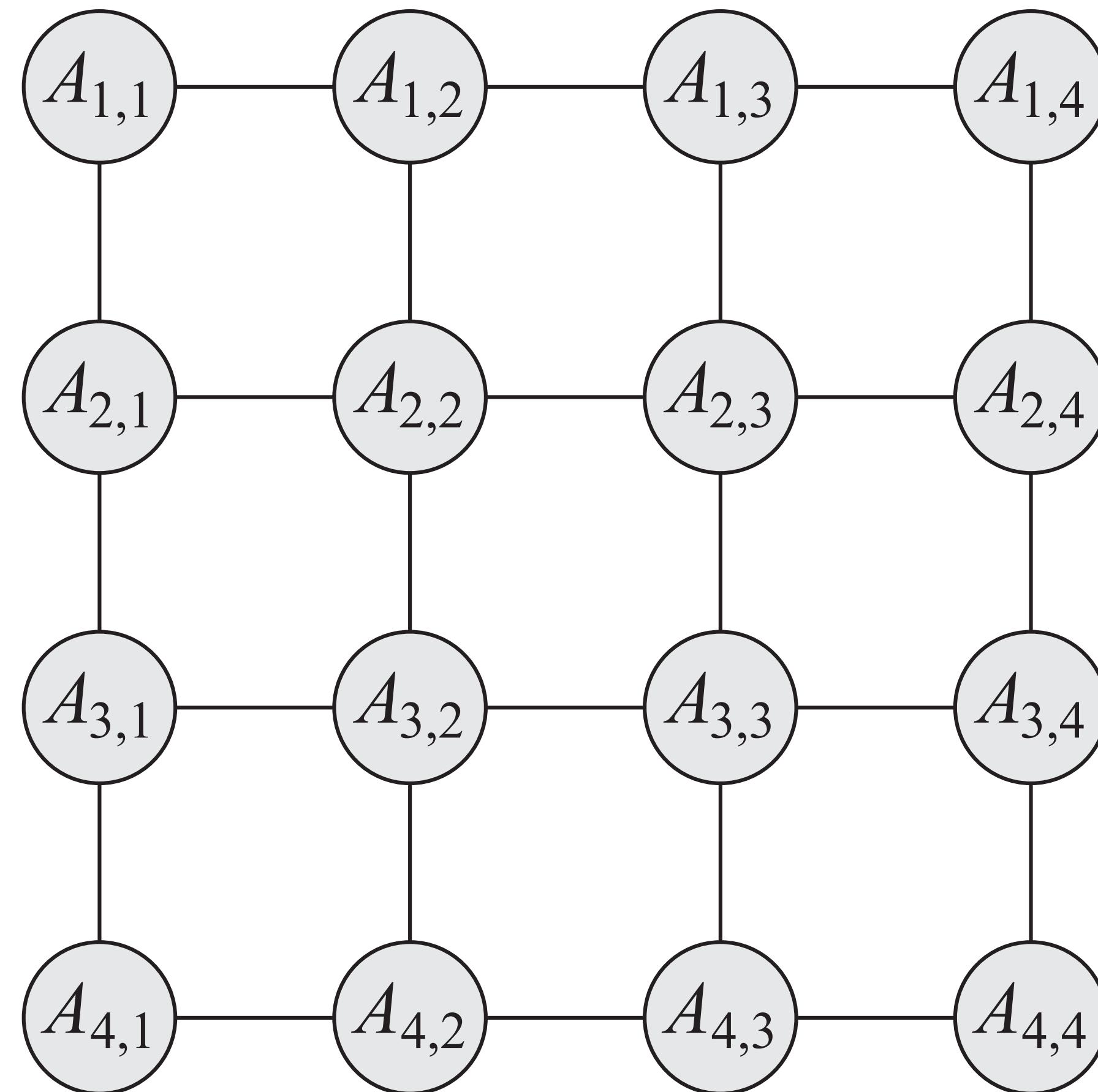
and each edge  $X_i - X_j$  is associated with a factor (aka potential)  $\phi_{ij}(X_i, X_j)$

# Pairwise Markov Networks

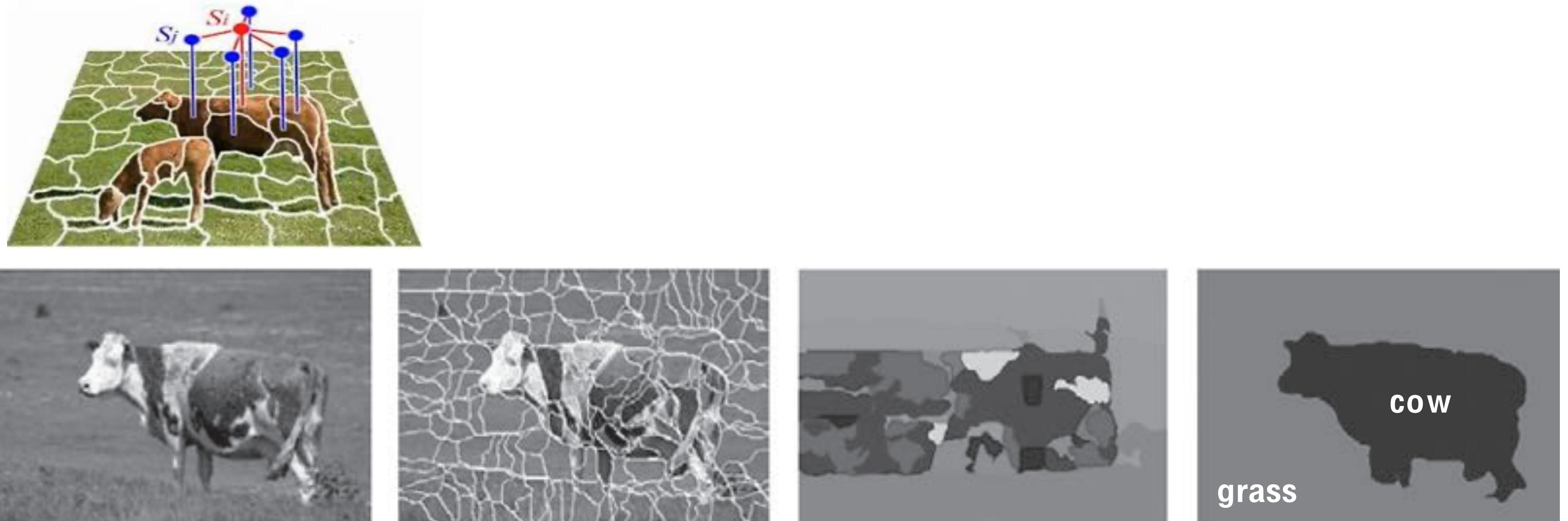
- A pairwise Markov network is an undirected graph whose nodes are random variables  $X_1, \dots, X_n$

and each edge  $X_i - X_j$  is associated with a factor (aka potential)  $\phi_{ij}(X_i, X_j)$

# Pairwise Markov Networks



# Pairwise Markov Networks



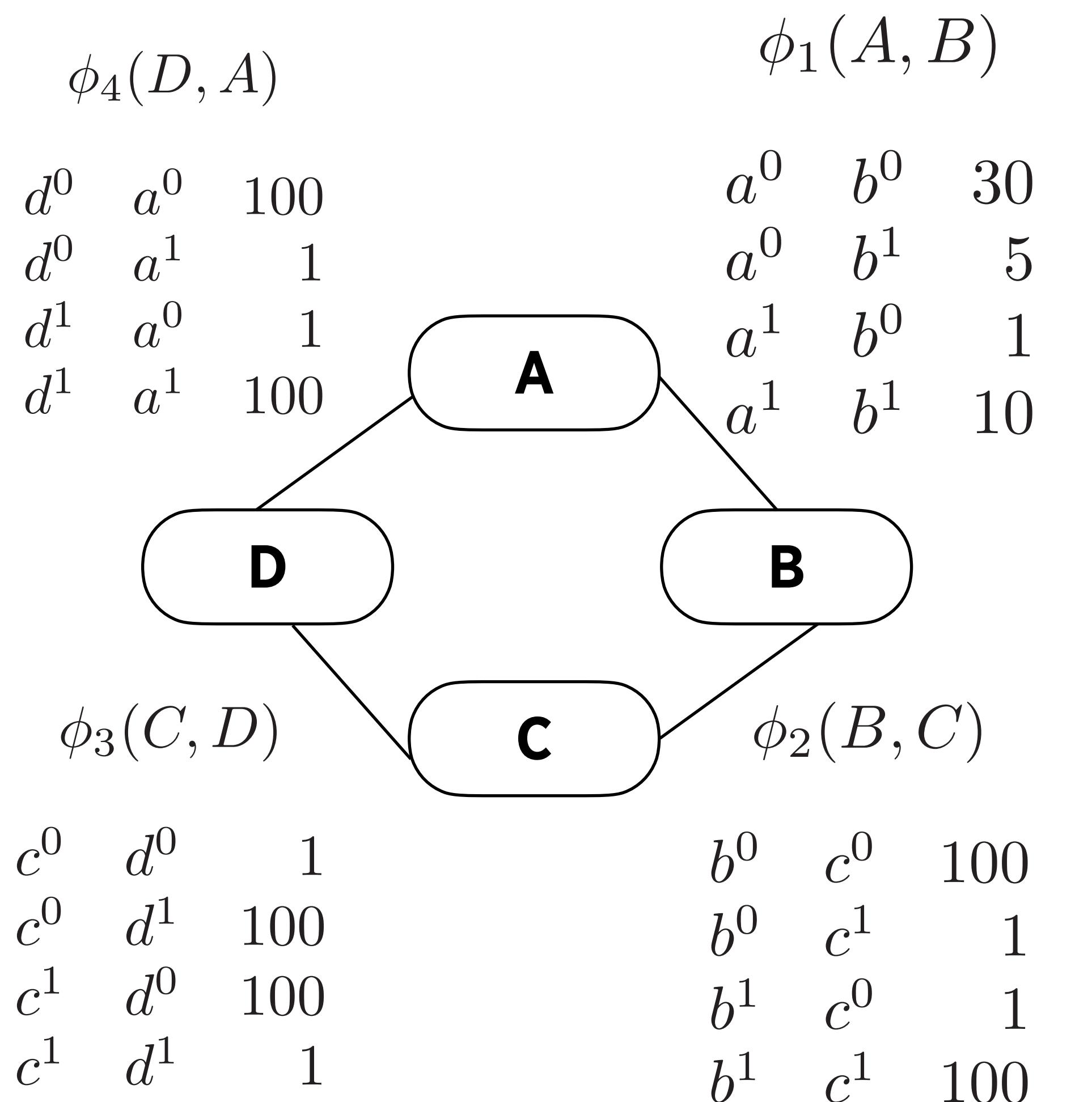
**examples of image segmentation results** (a) The original image. (b) An oversegmentation known as superpixels; each superpixel is associated with a random variable that designates its segment assignment. The use of superpixels reduces the size of the problems. (c) Result of segmentation using node potentials alone, so that each superpixel is classified independently. (d) Result of segmentation using a pairwise Markov network encoding interactions between adjacent superpixels.

# Summary

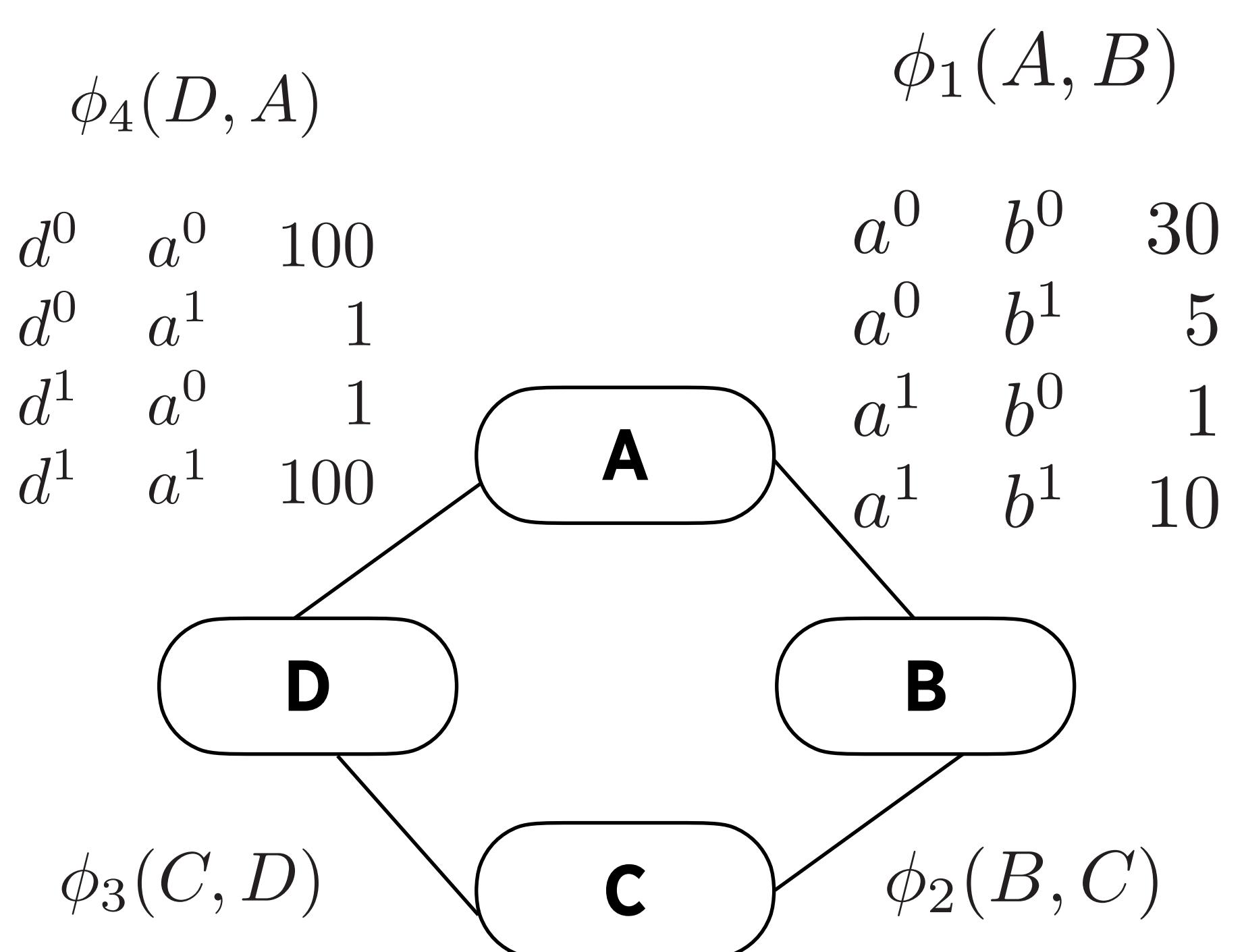
- **Bayesian networks**
- Factors
- Markov networks

# **Belief Propagation Algorithm**

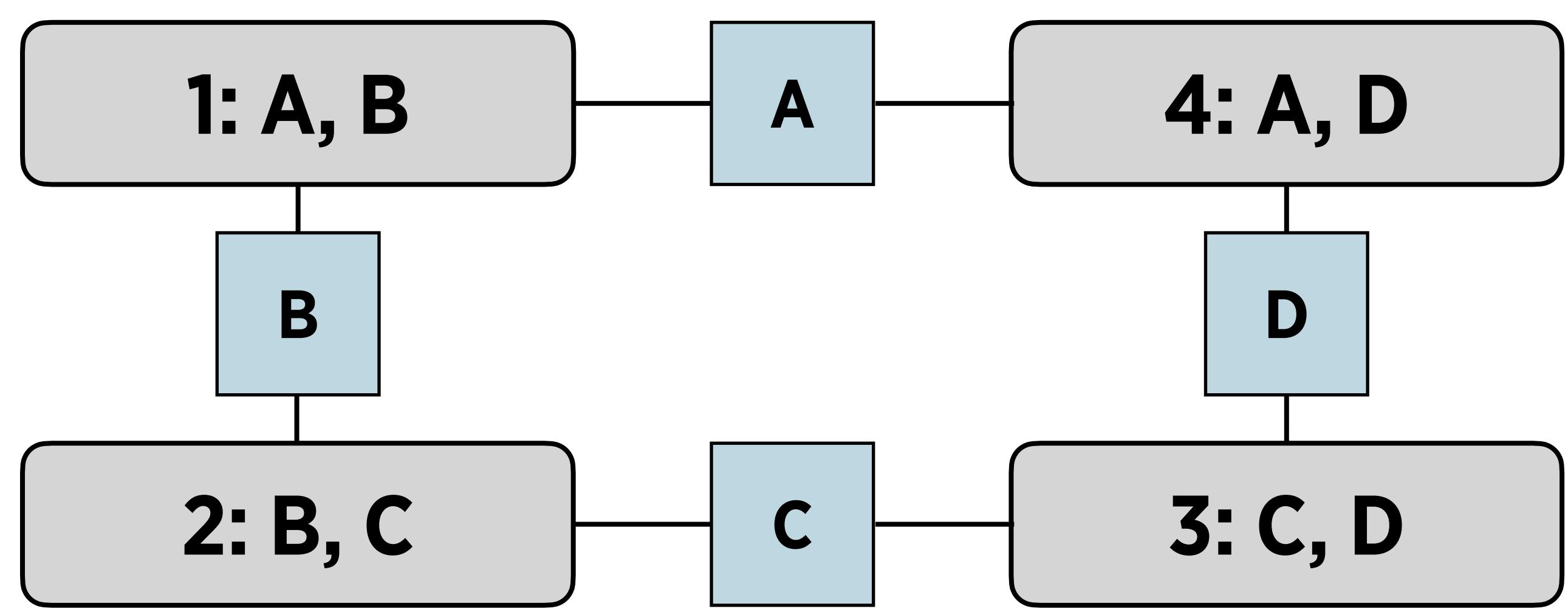
# Cluster Graph



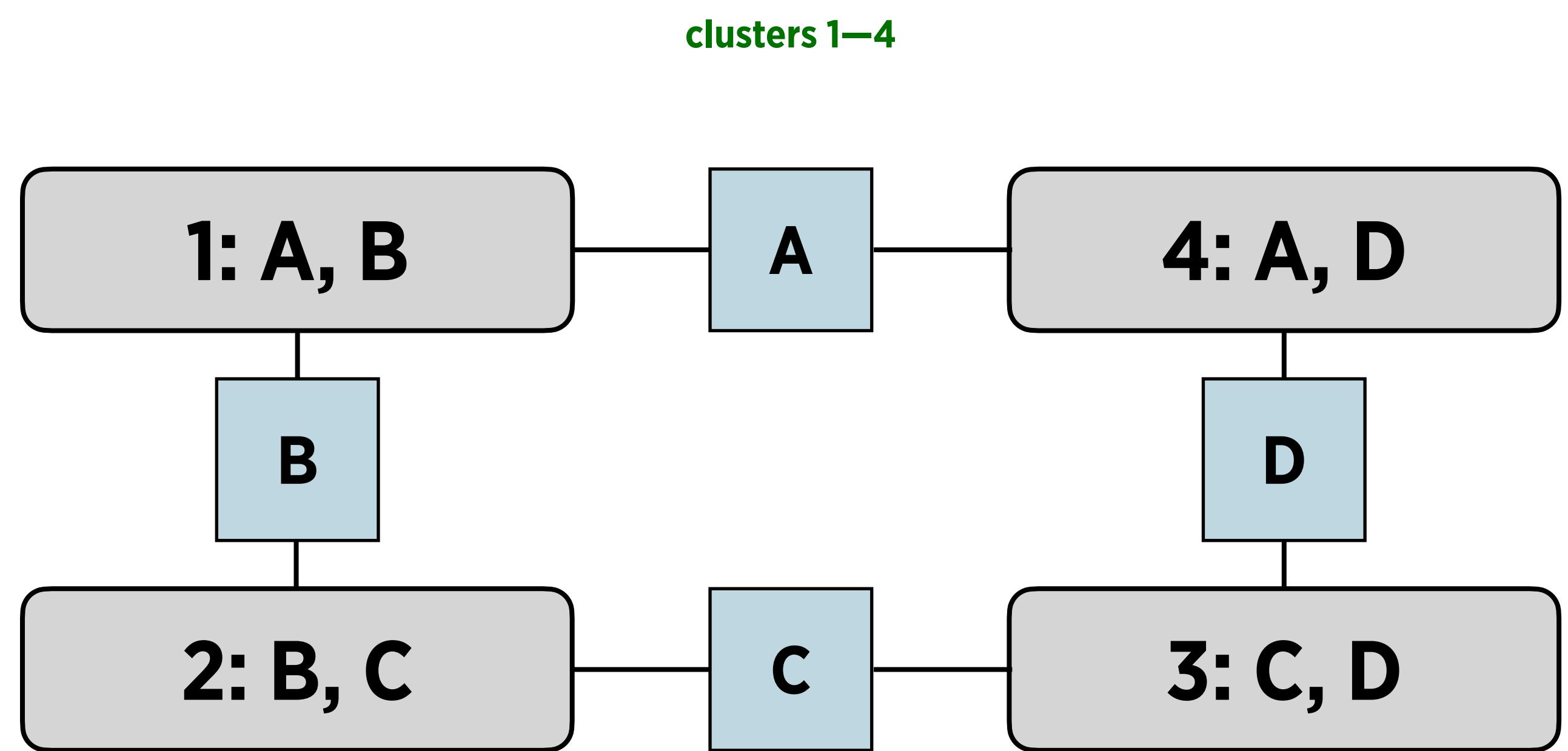
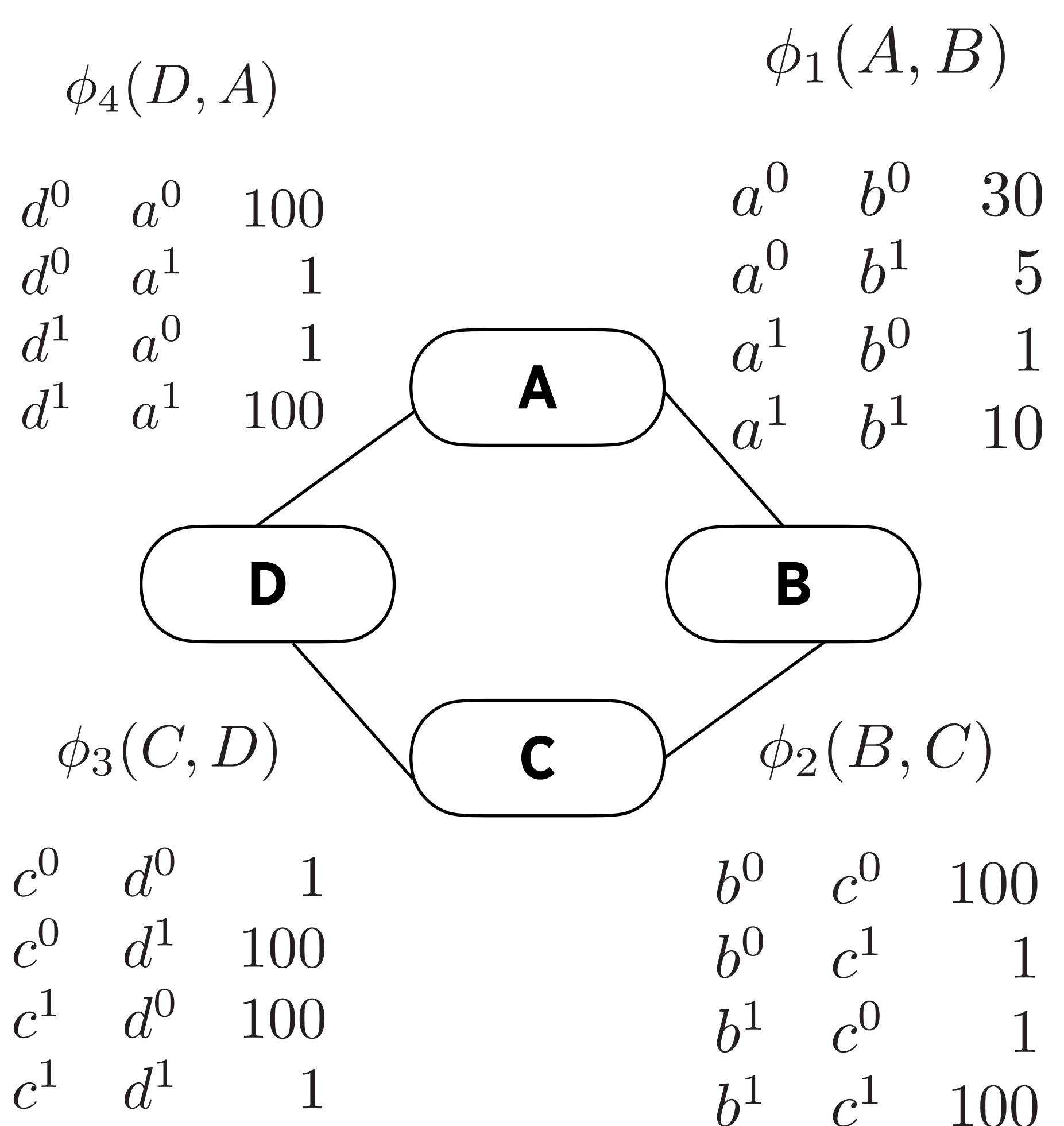
# Cluster Graph



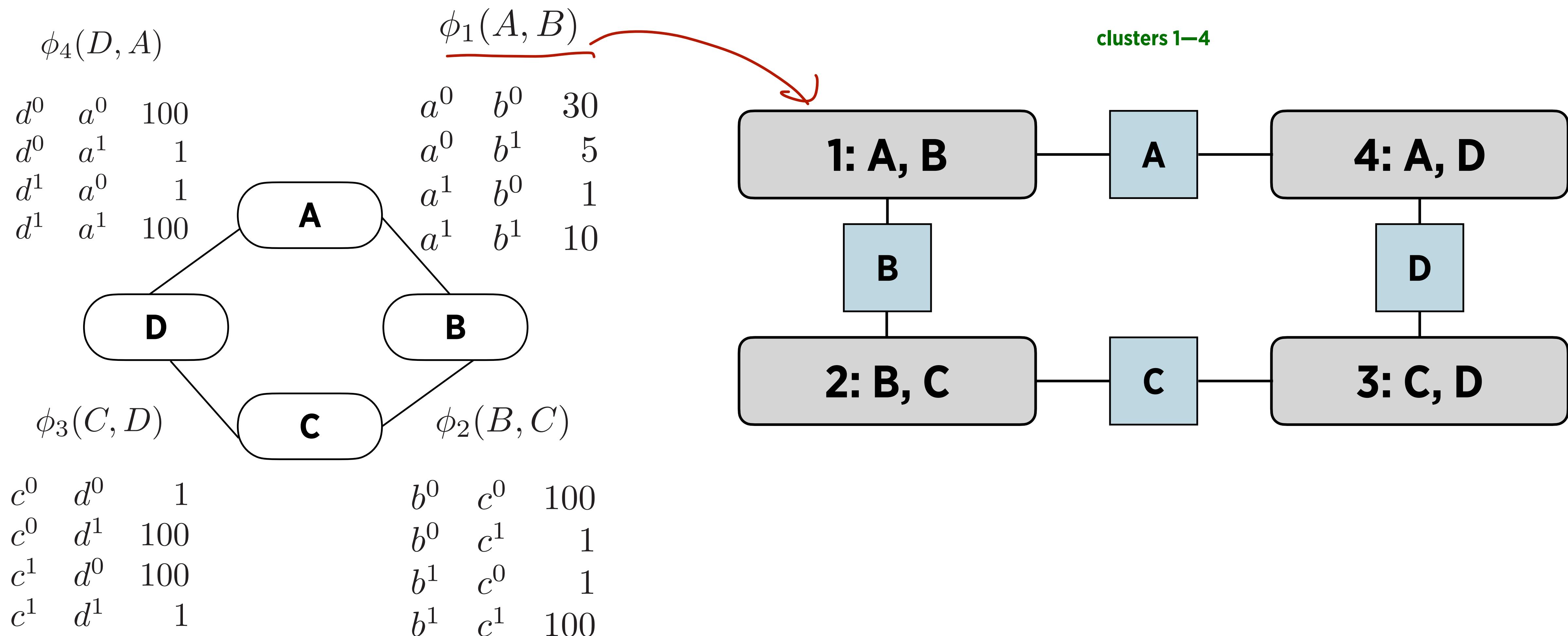
$c^0$	$d^0$	1	$b^0$	$c^0$	100
$c^0$	$d^1$	100	$b^0$	$c^1$	1
$c^1$	$d^0$	100	$b^1$	$c^0$	1
$c^1$	$d^1$	1	$b^1$	$c^1$	100



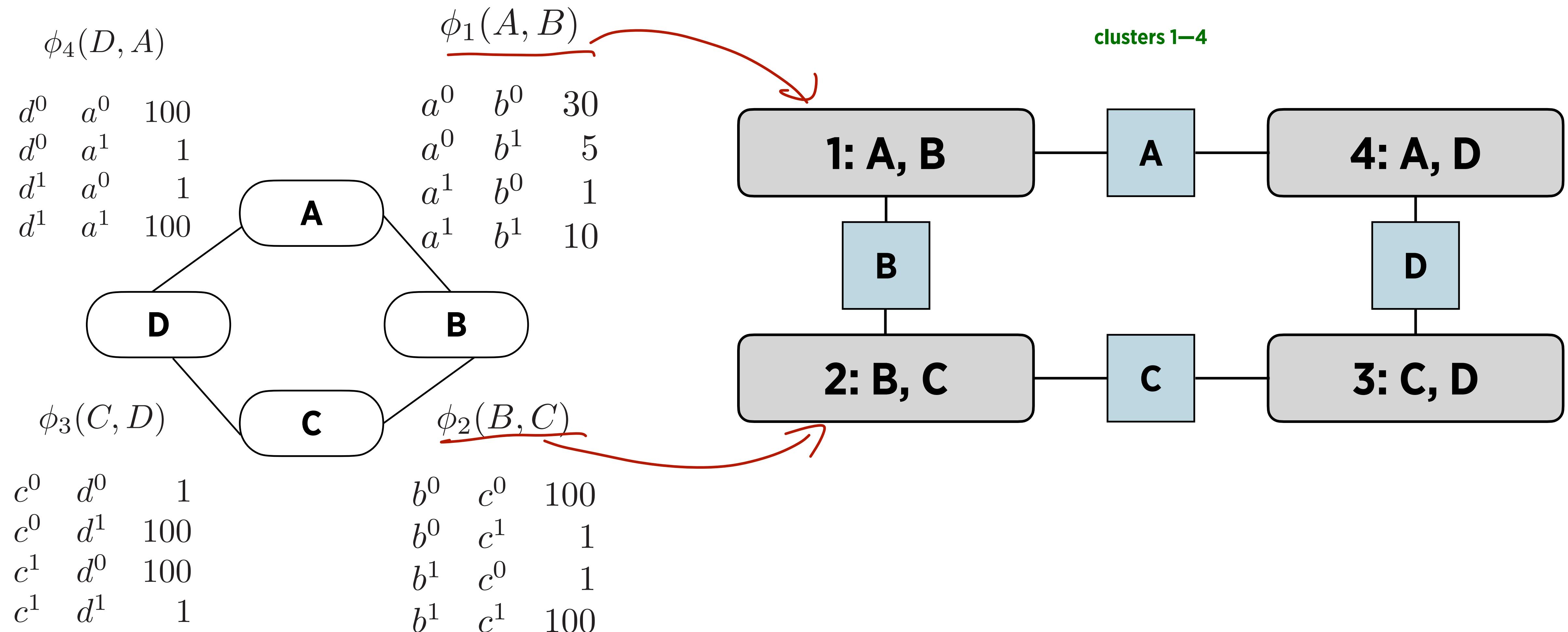
# Cluster Graph



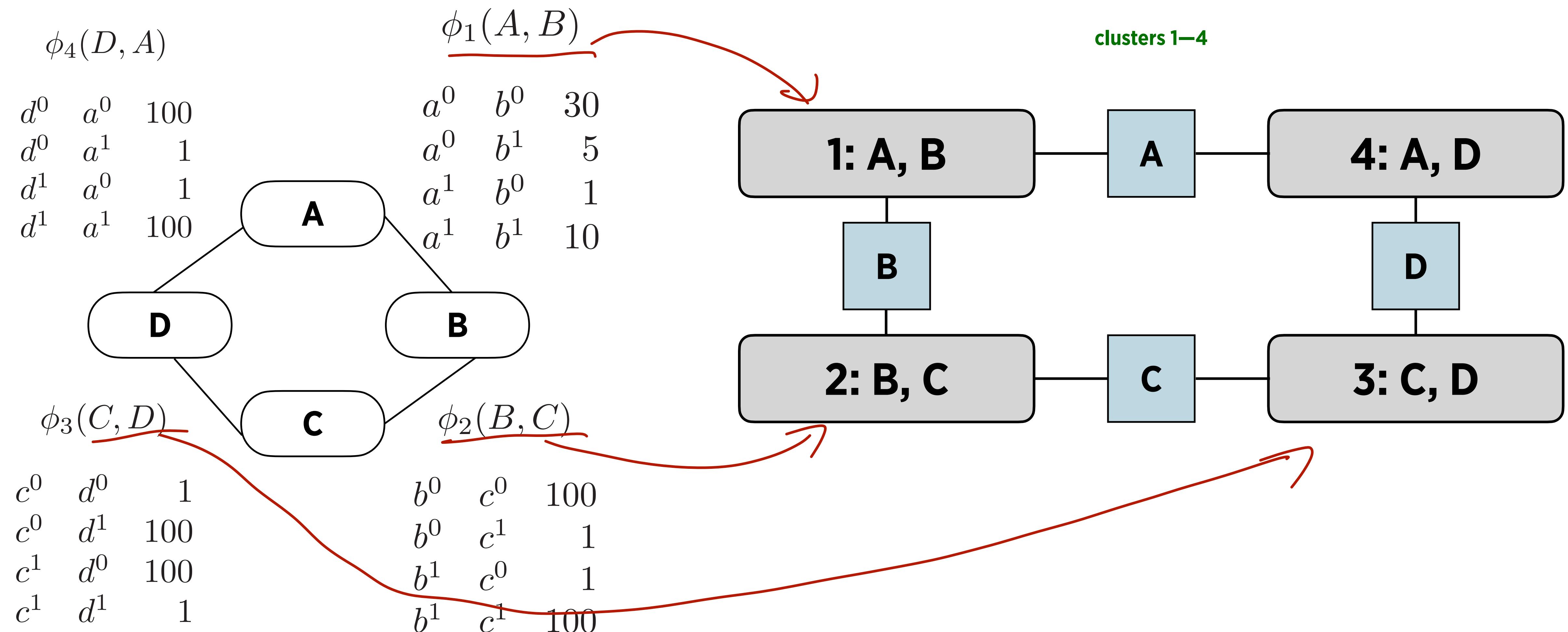
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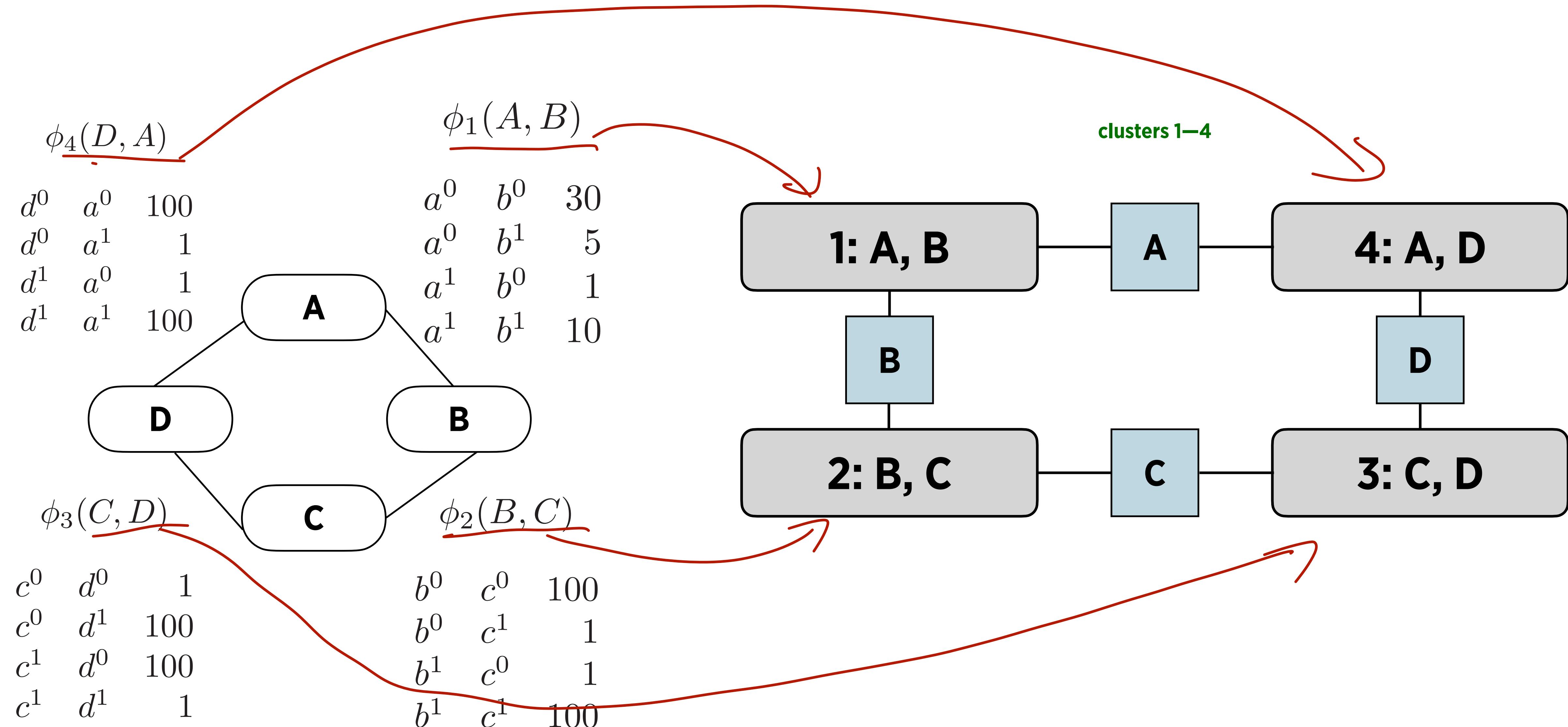
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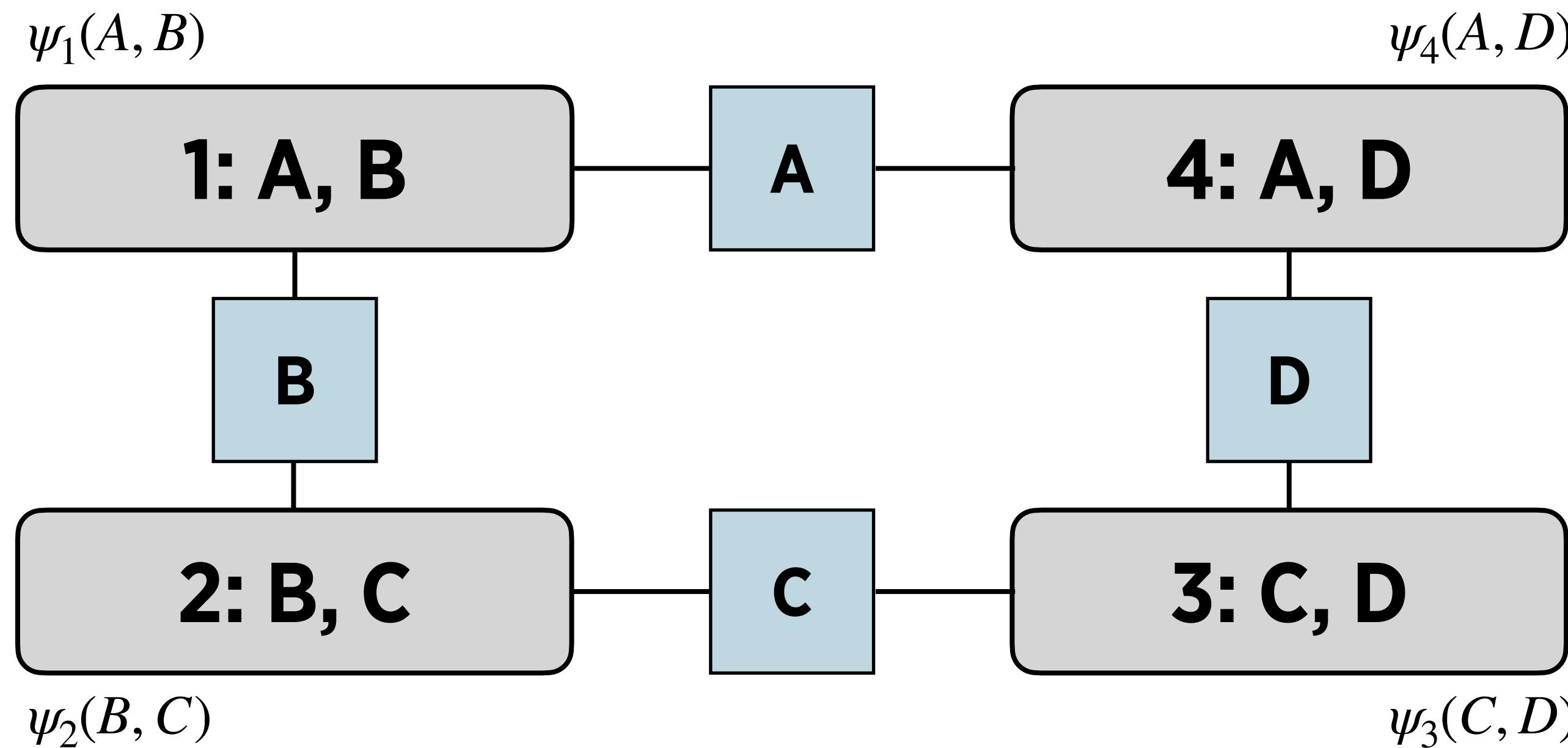
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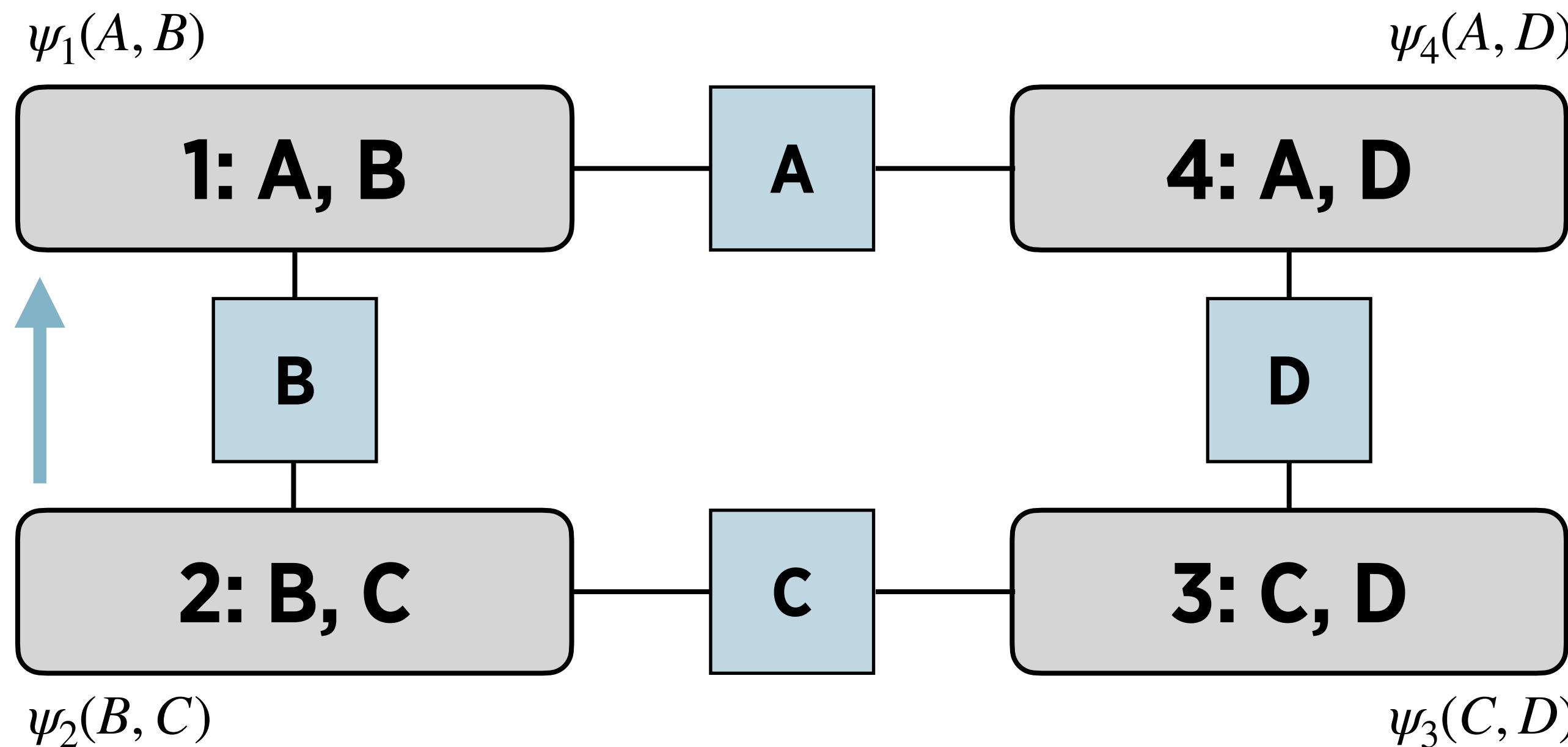
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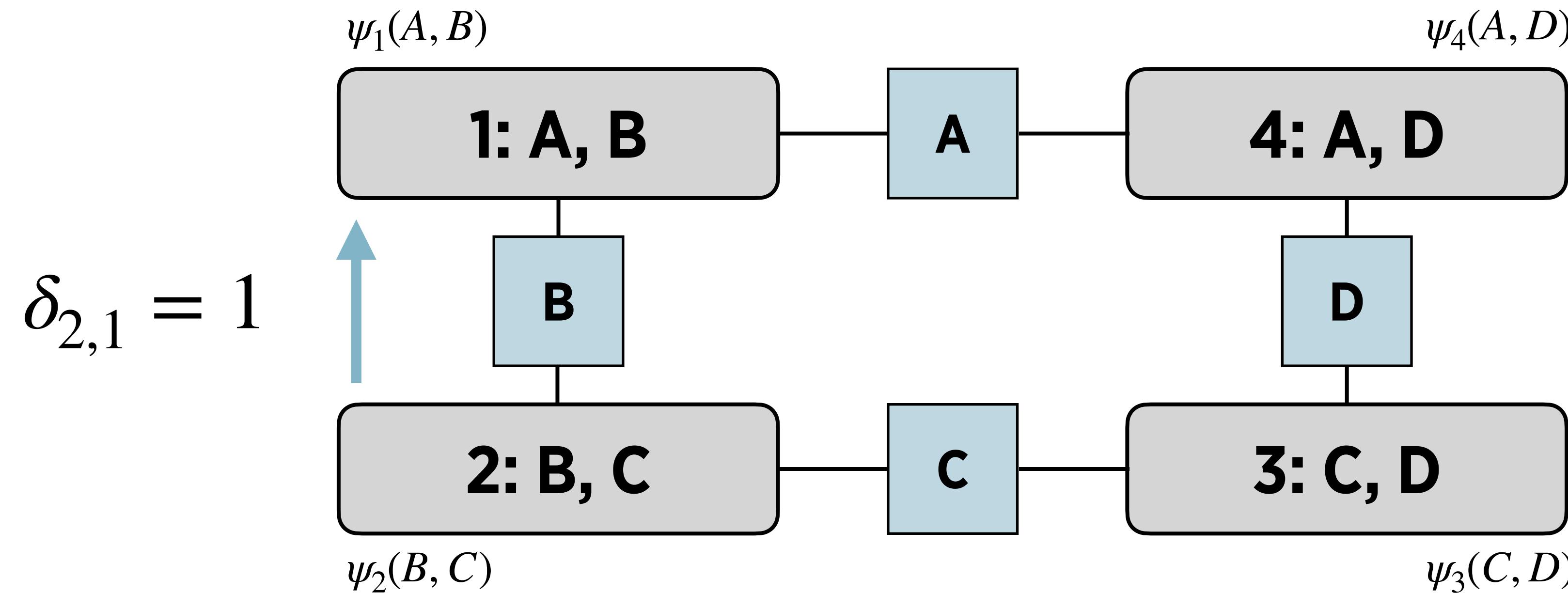
# Passing messages



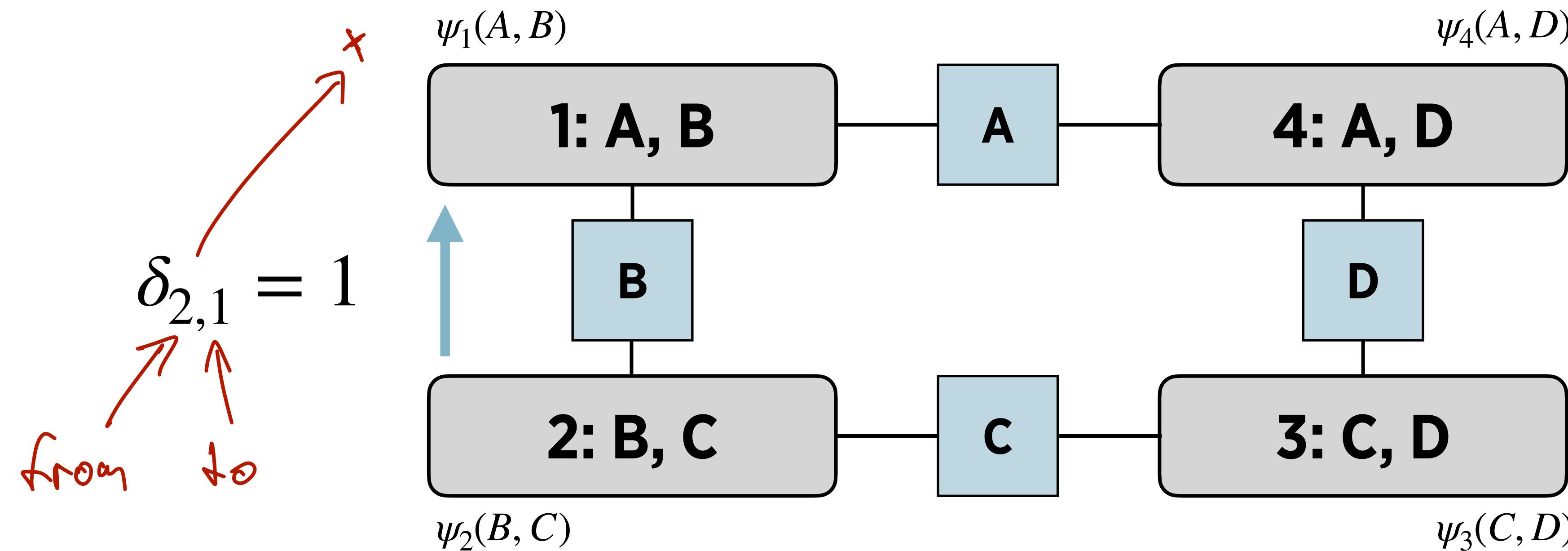
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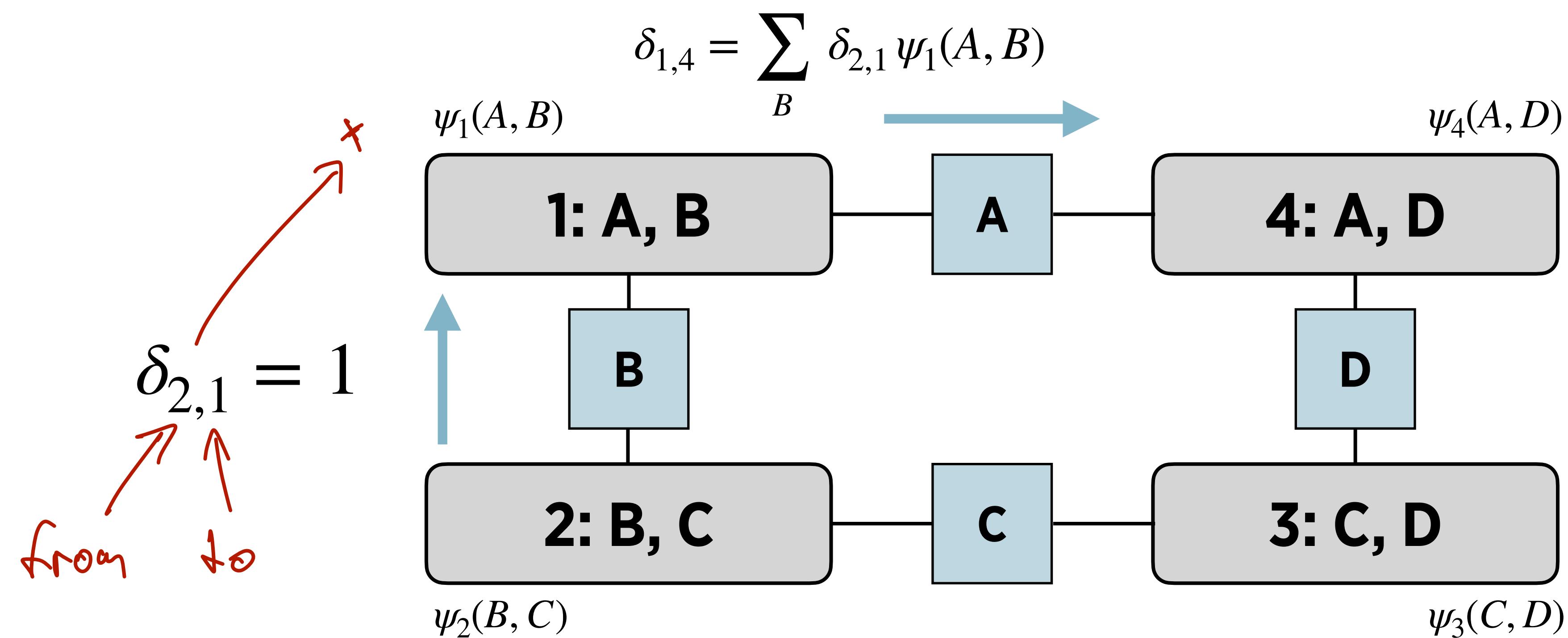
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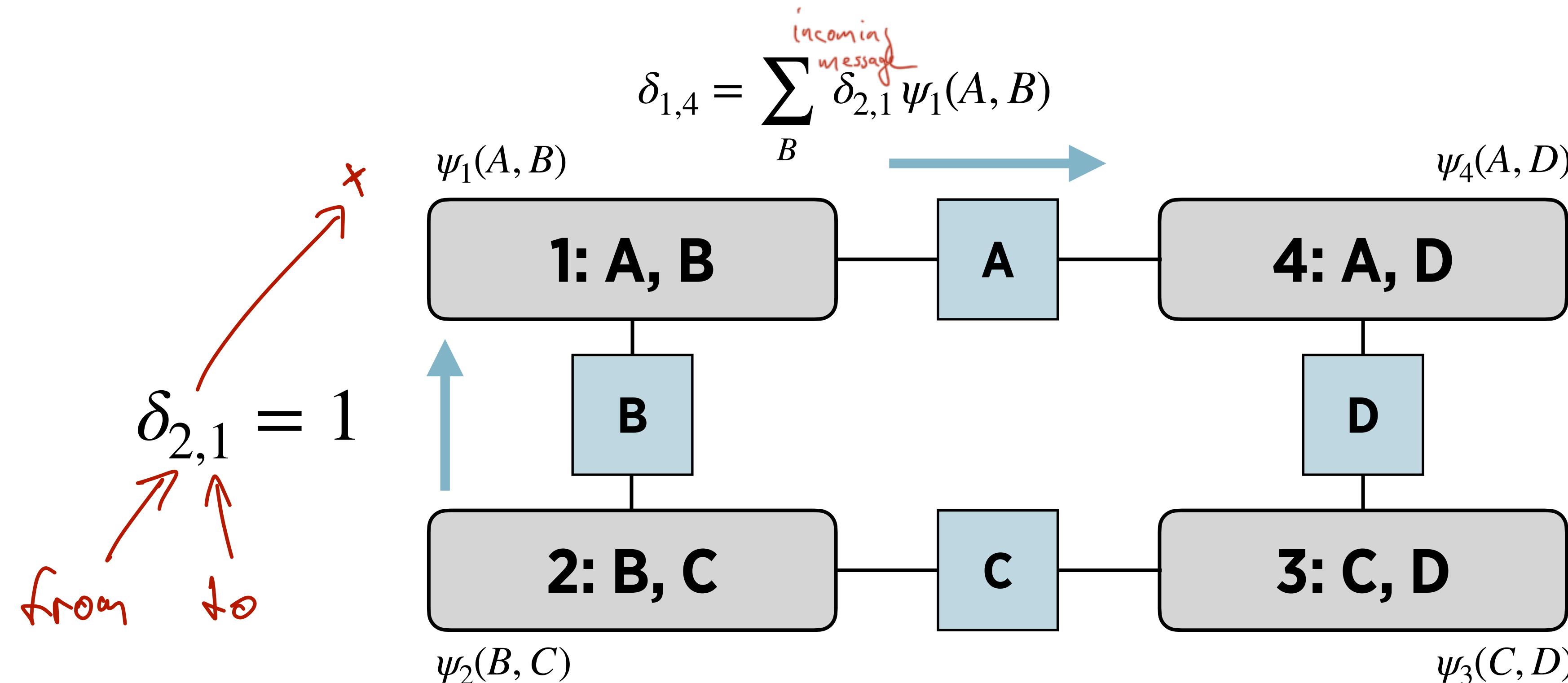
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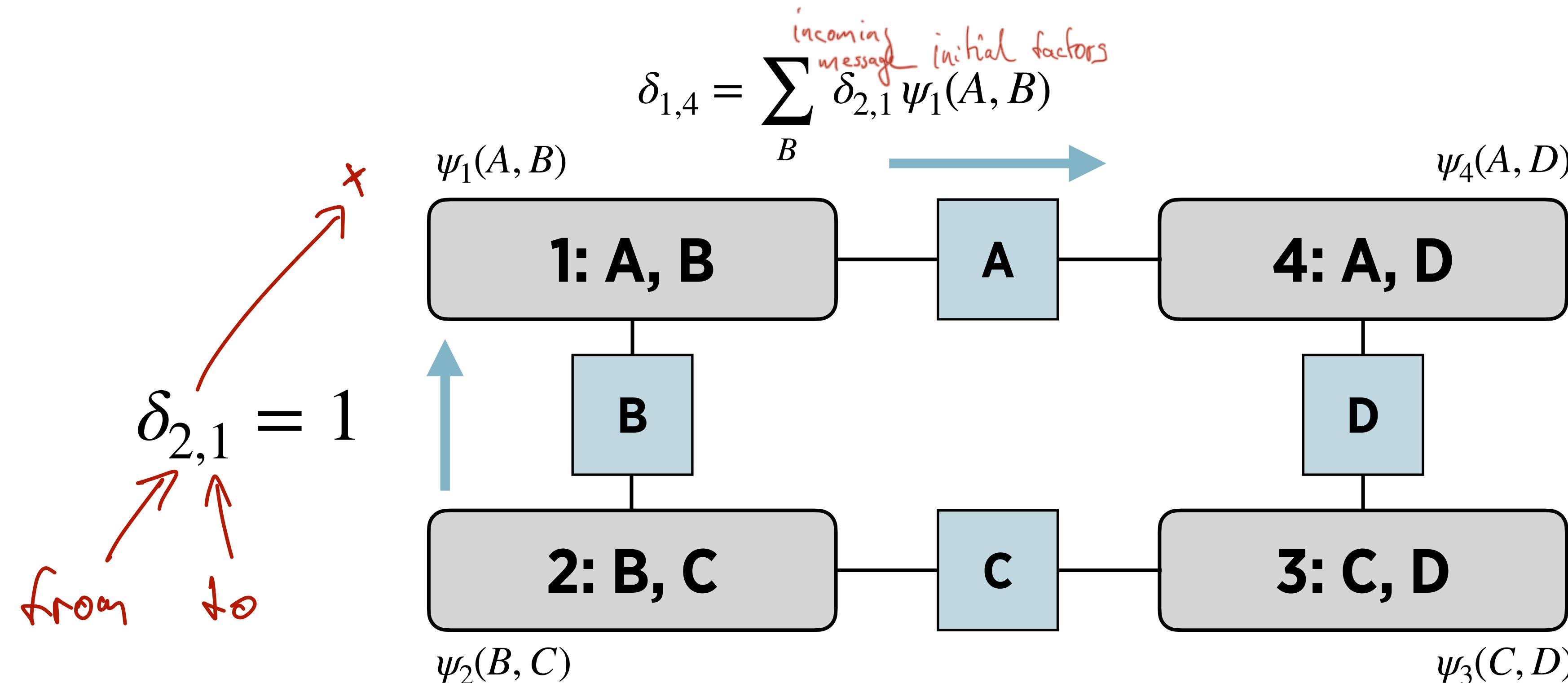
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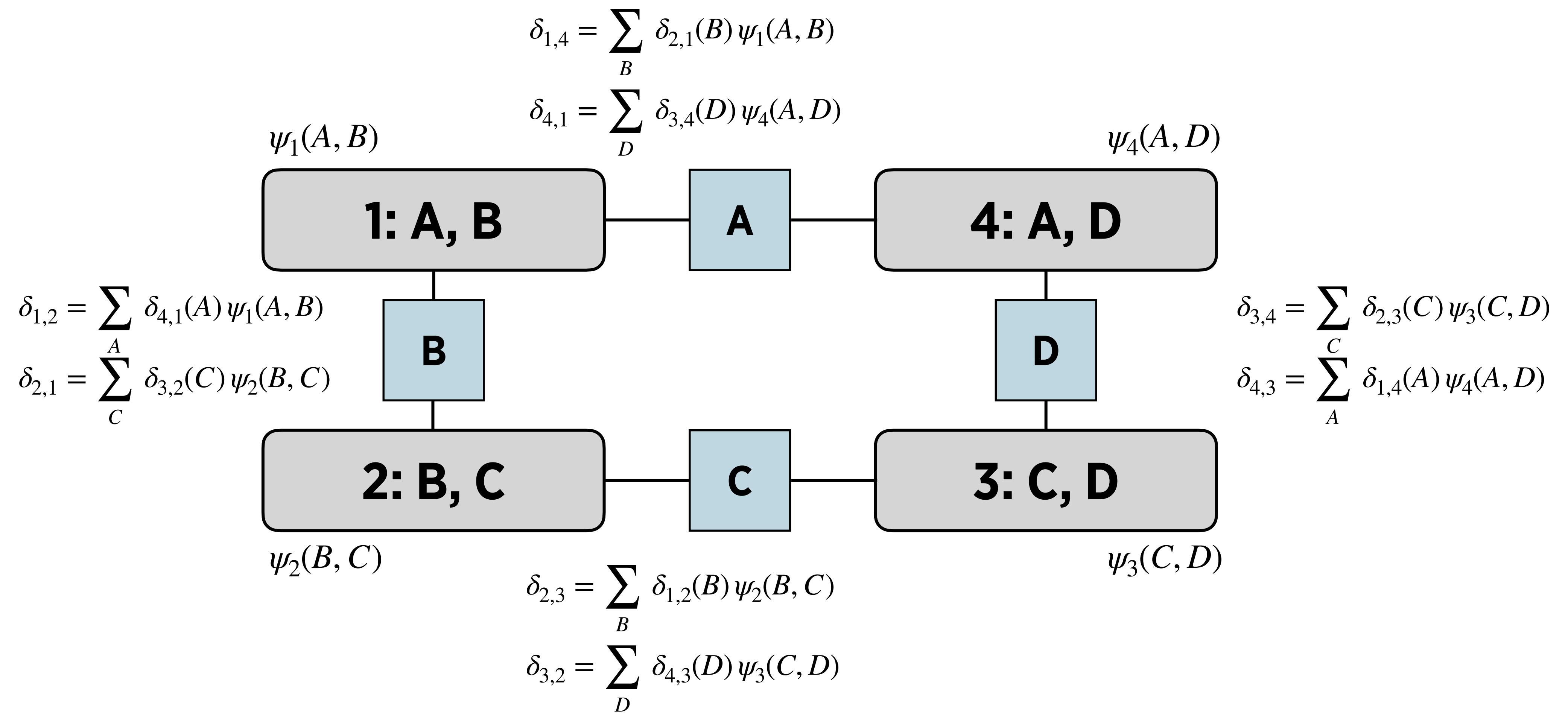
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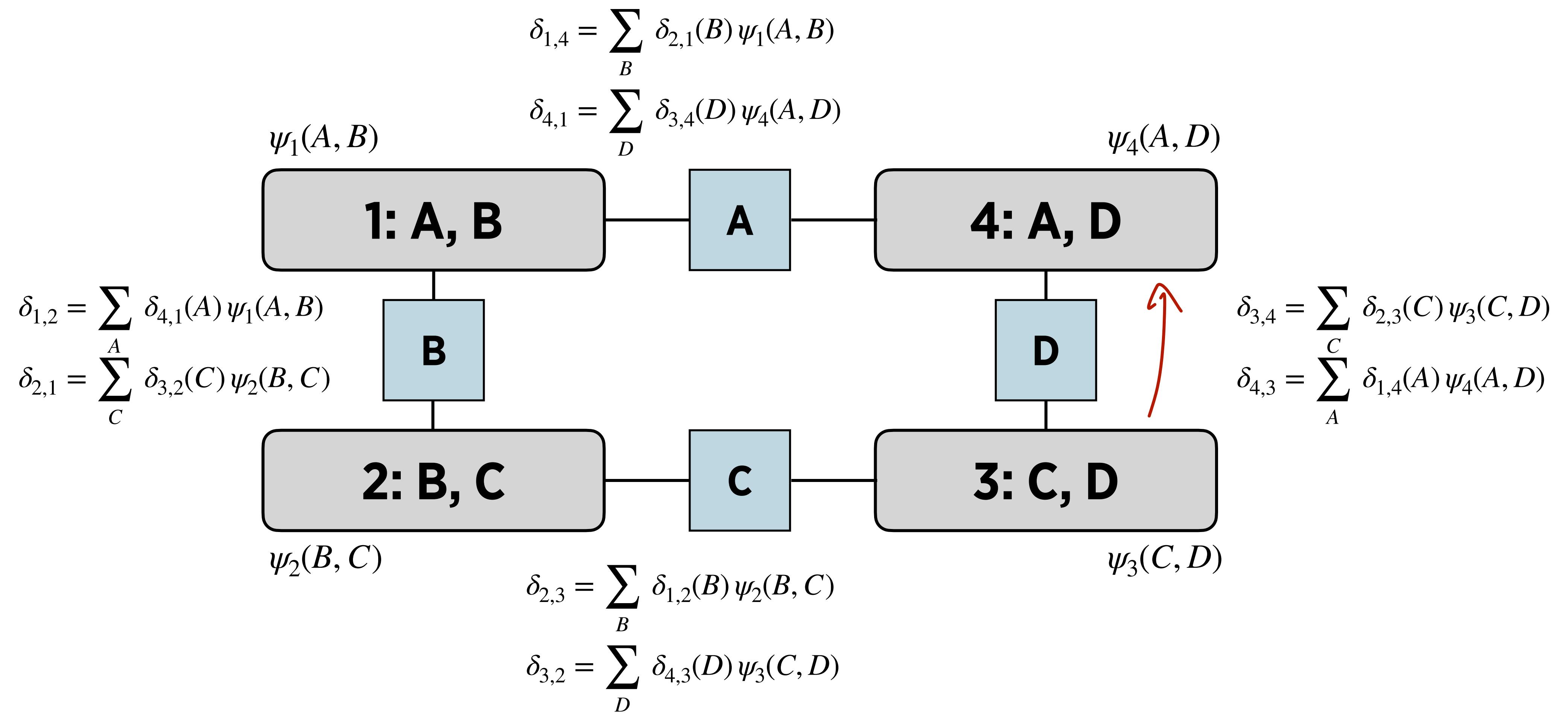
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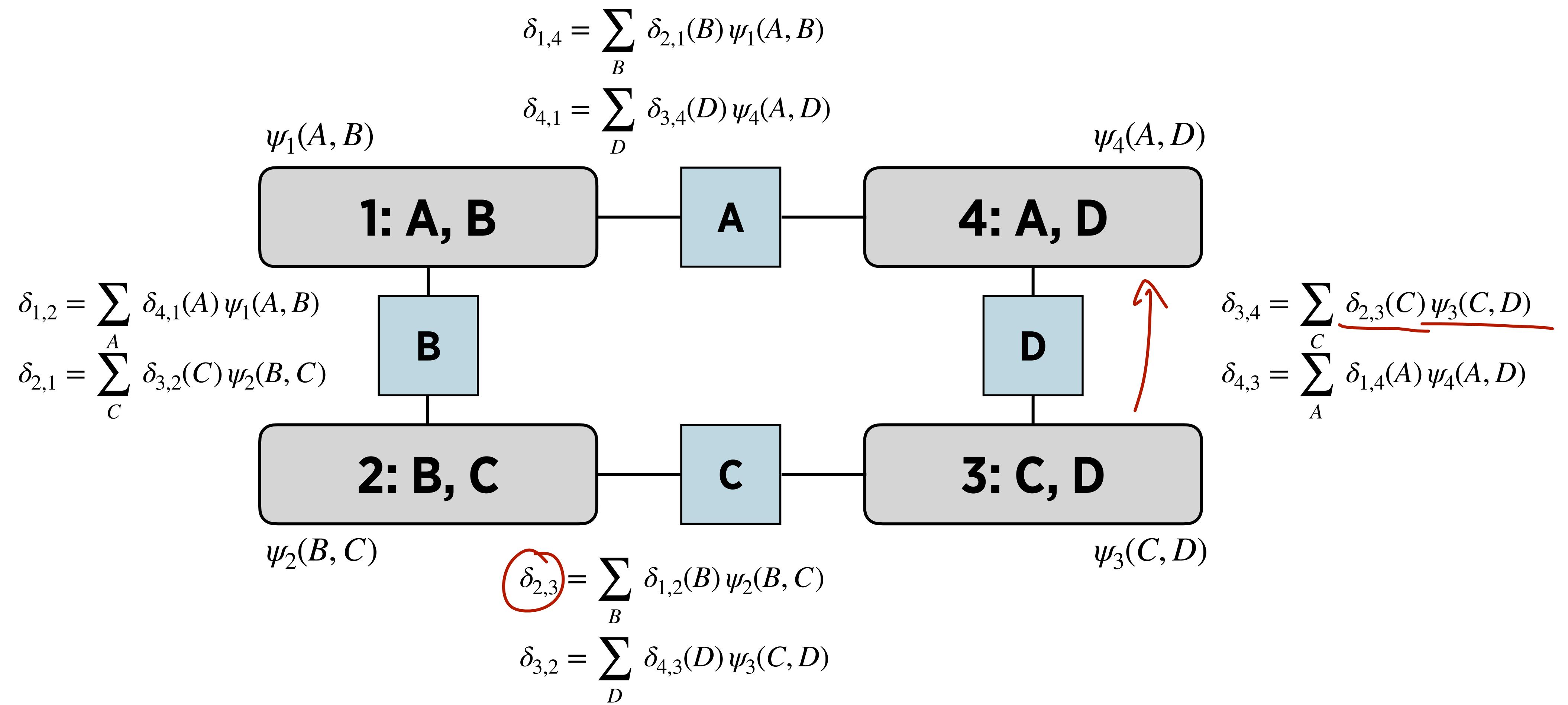
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# Cluster Graphs

# Cluster Graphs

- Undirected graph such that:
  - Nodes are clusters  $C_i \subseteq \{X_1, \dots, X_n\}$
  - Edge between  $C_i$  and  $C_j$  associated with sepset  $S_{i,j} \subseteq C_i \cap C_j$ 
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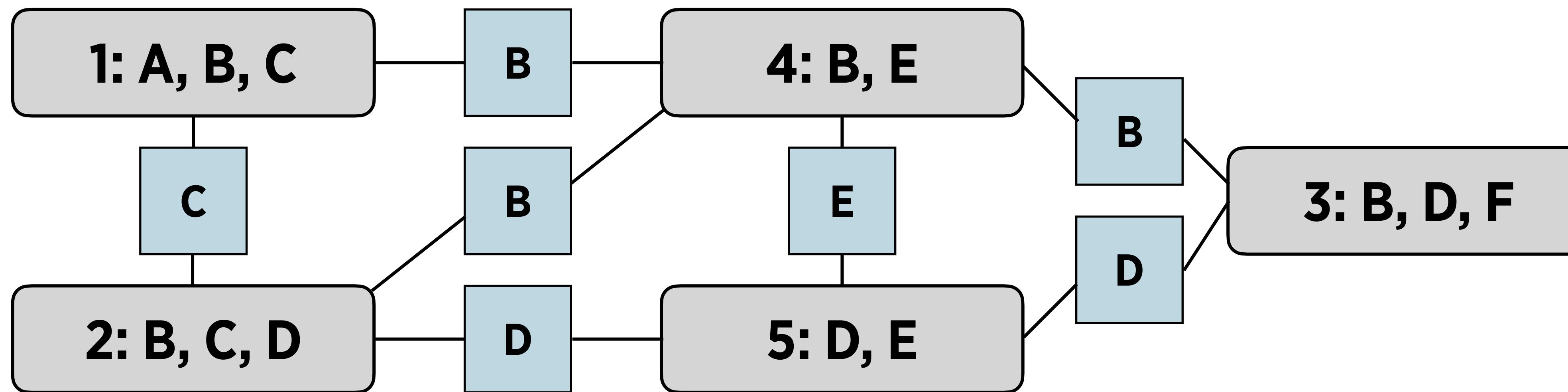
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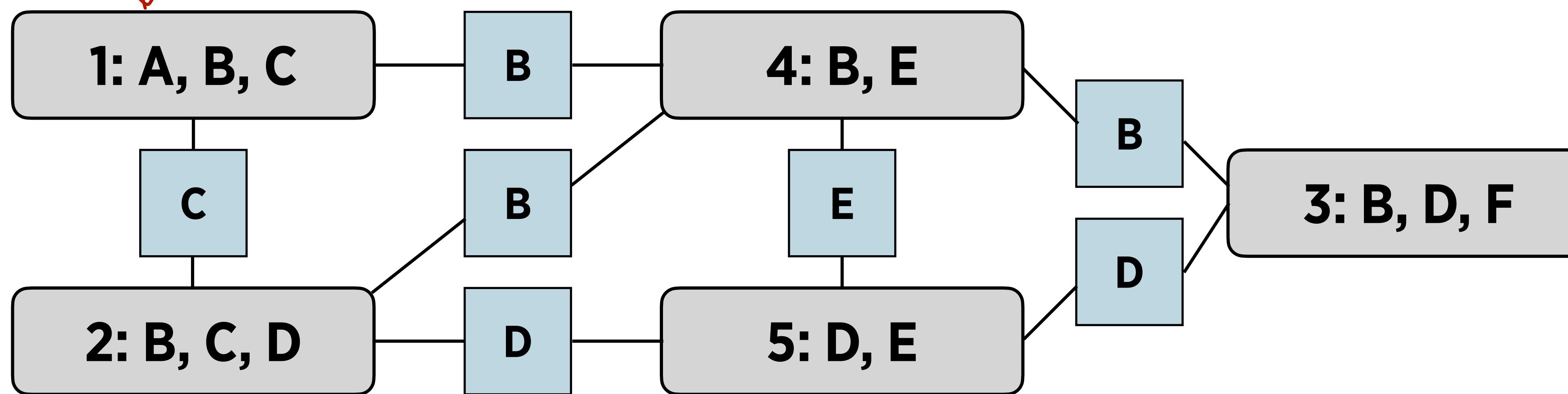
# Example cluster graph

$\phi_1(A, B, C), \phi_2(B, C), \phi_3(B, D), \phi_4(D, E), \phi_5(B, E), \phi_6(B, D), \phi_7(B, D, F)$

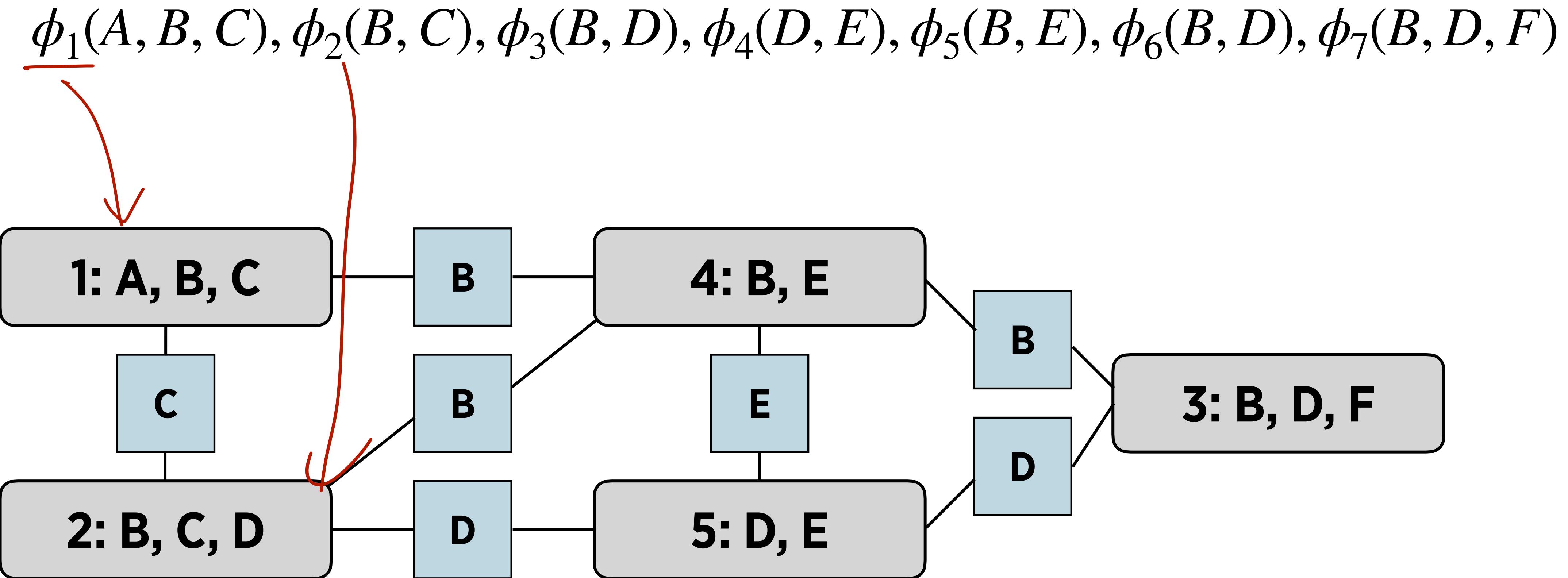


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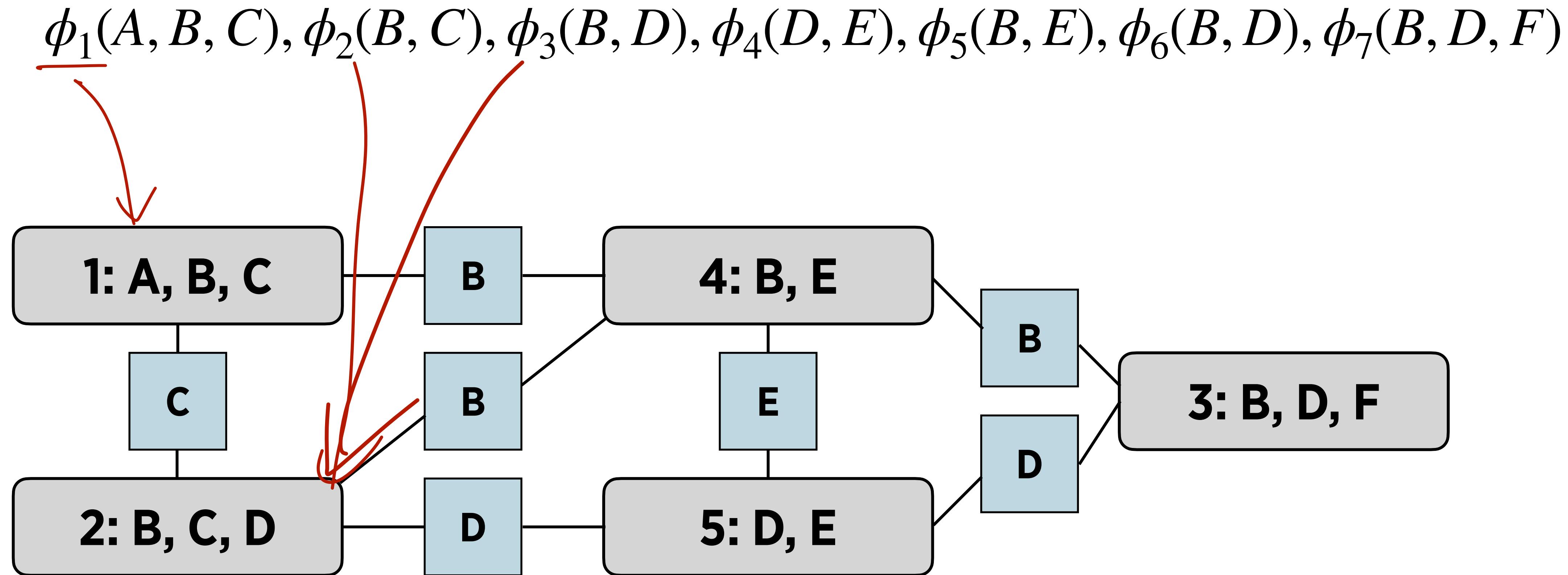
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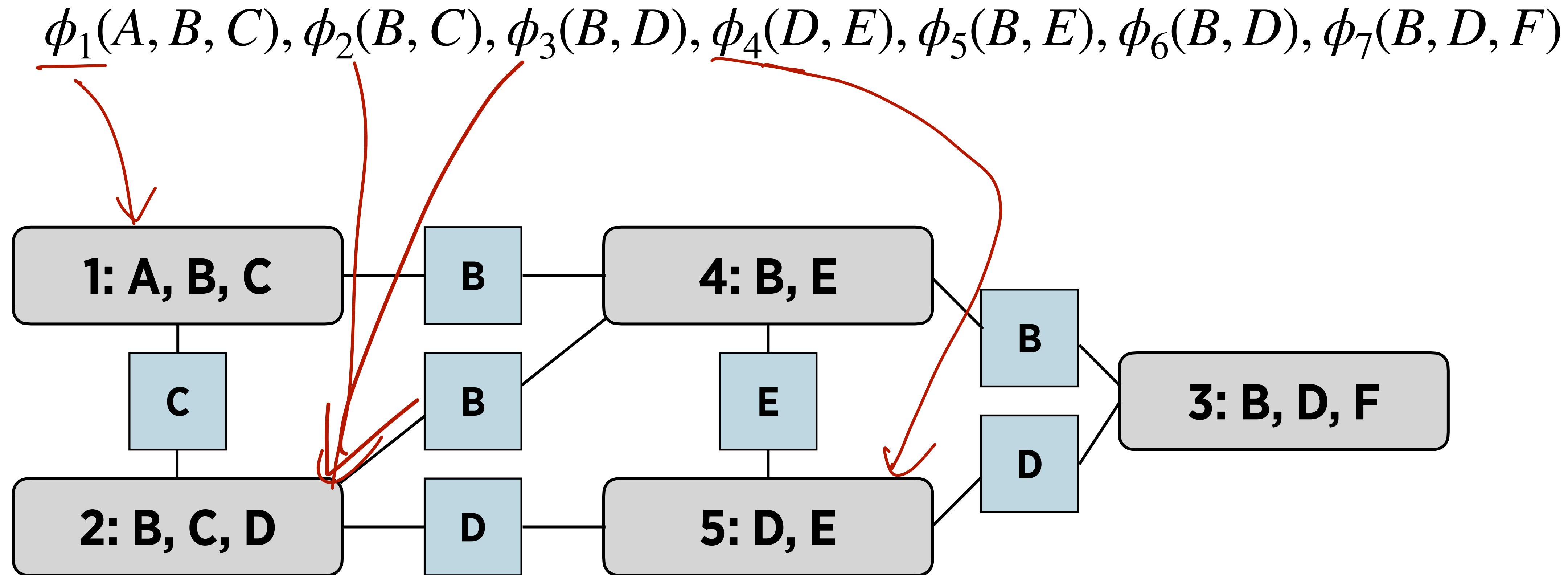
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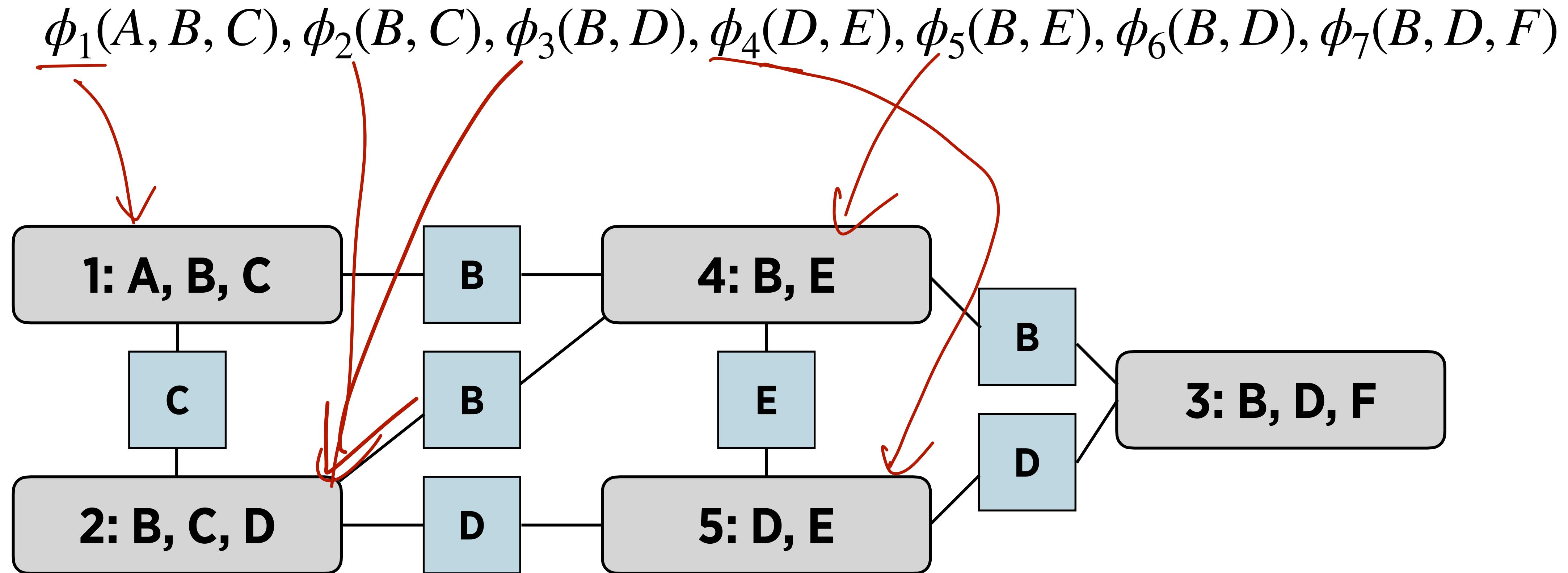
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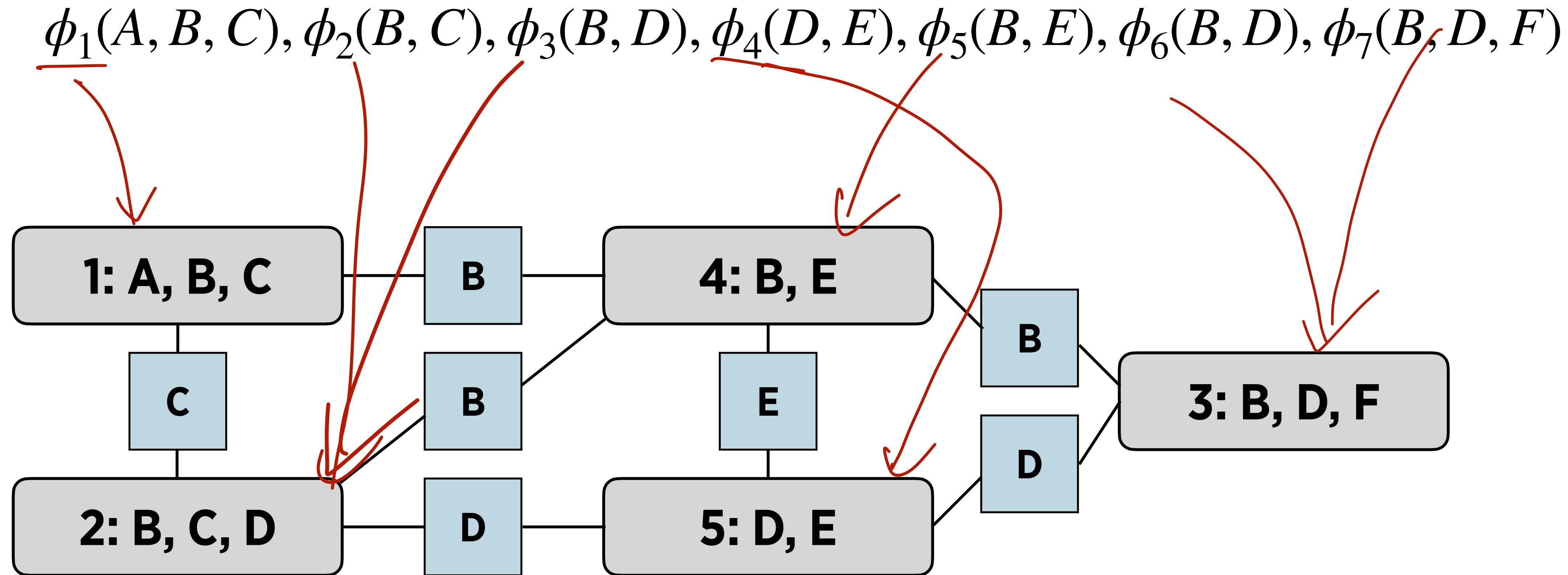
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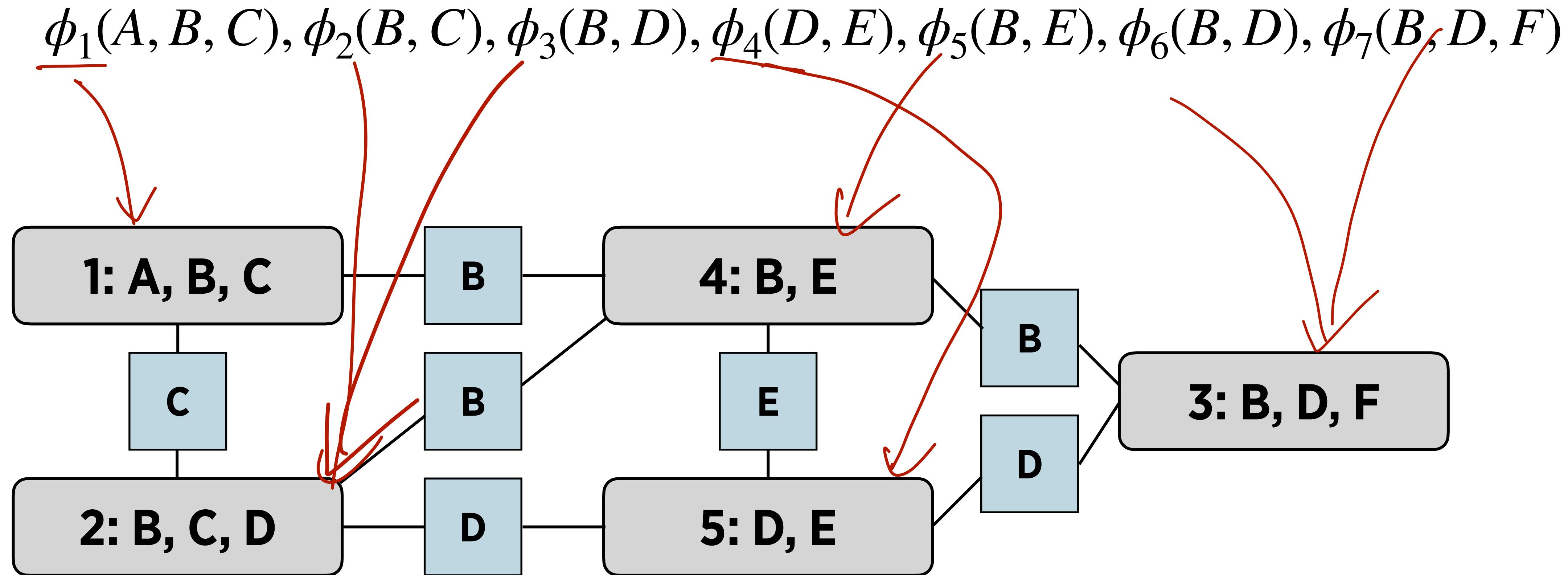
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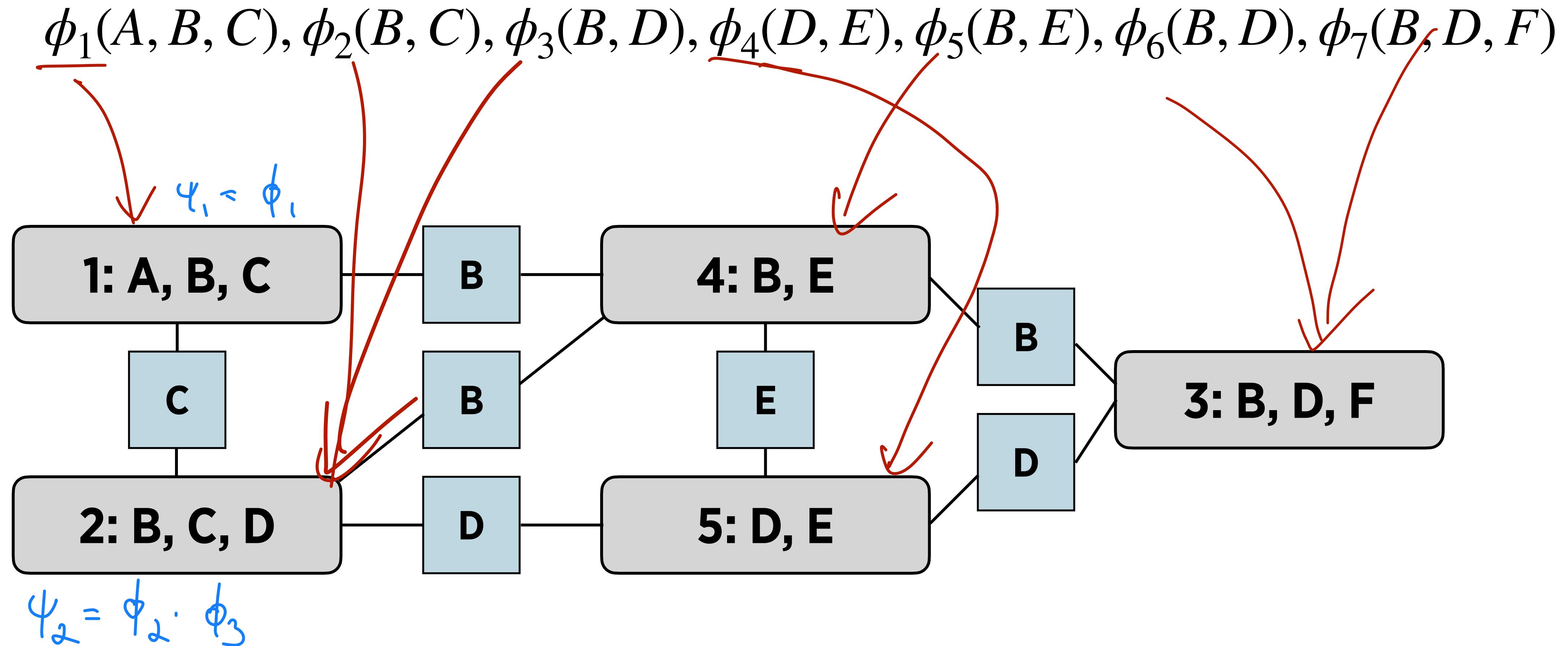


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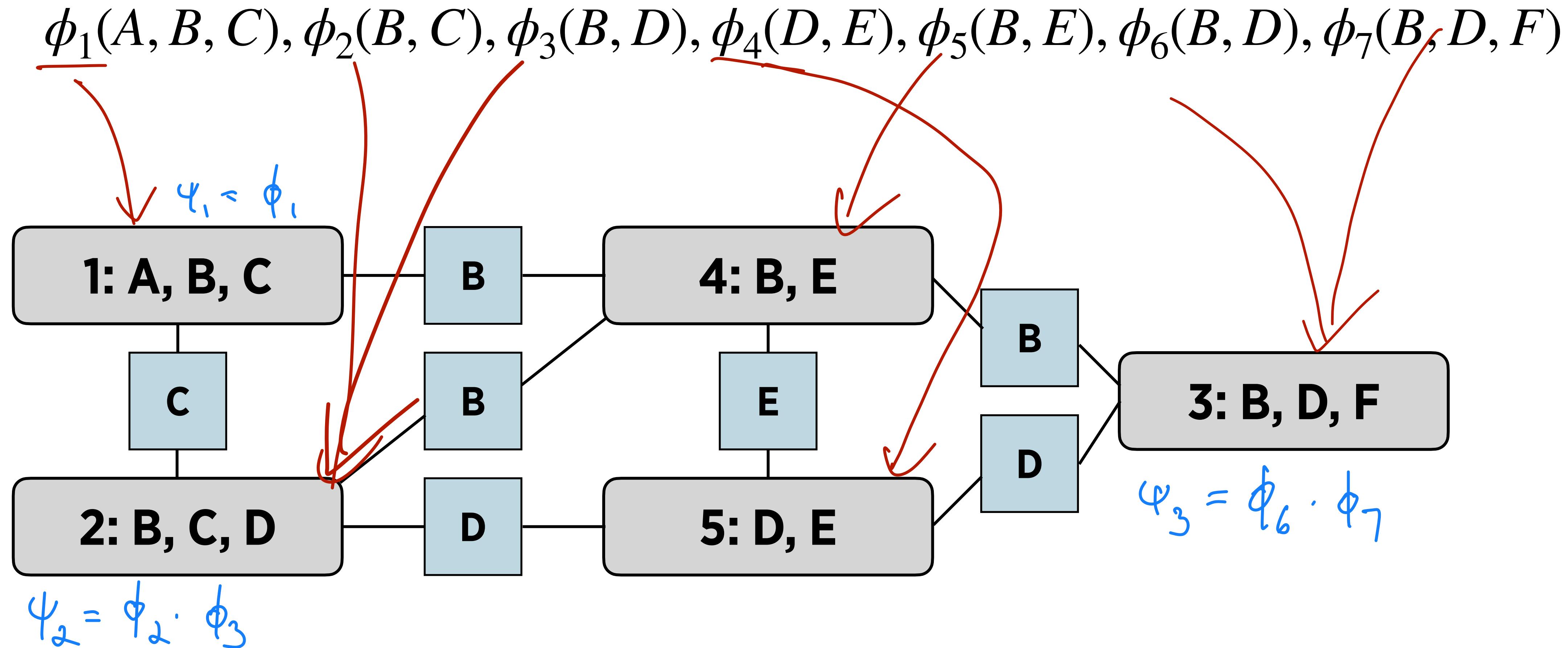


$$\psi_2 = \phi_2 \cdot \phi_3$$

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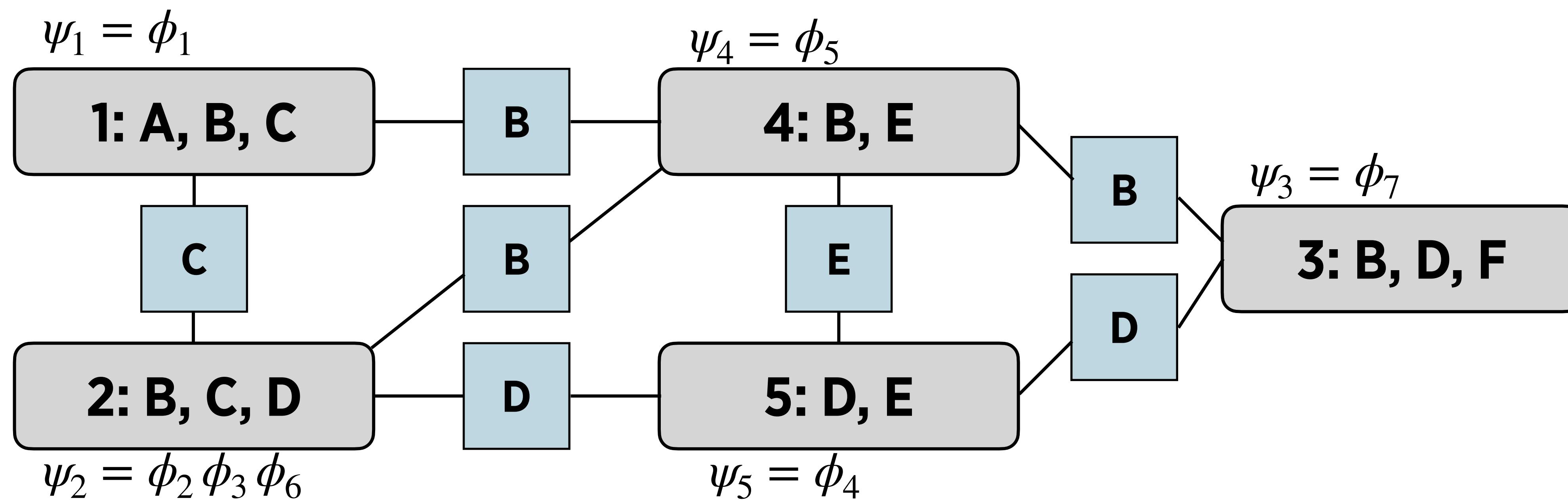


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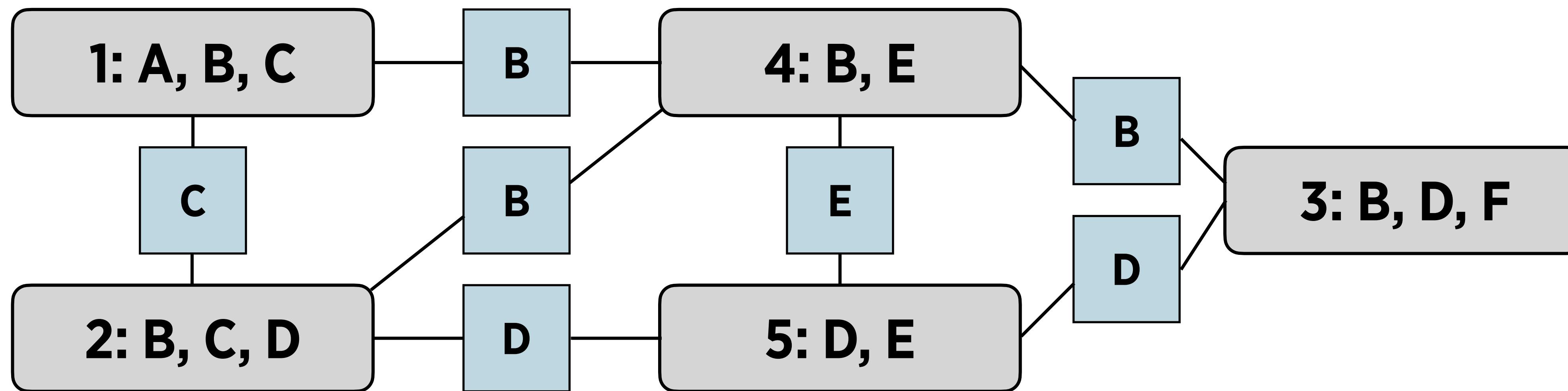
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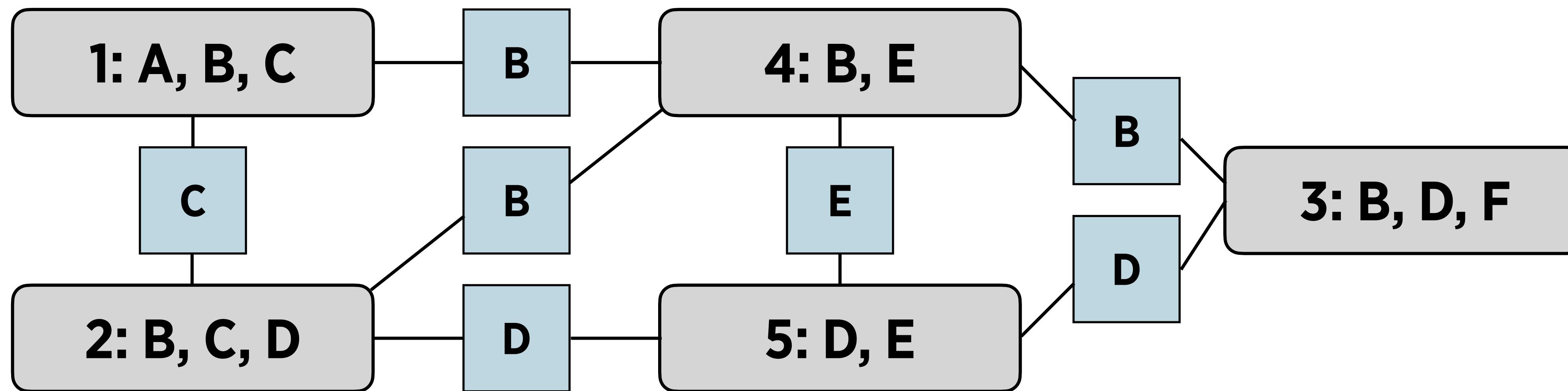
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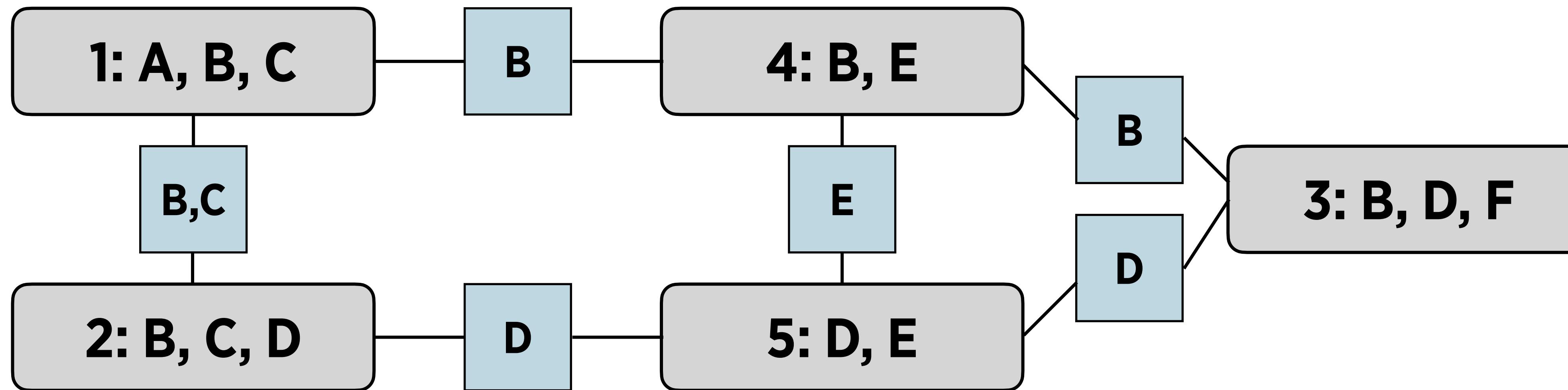
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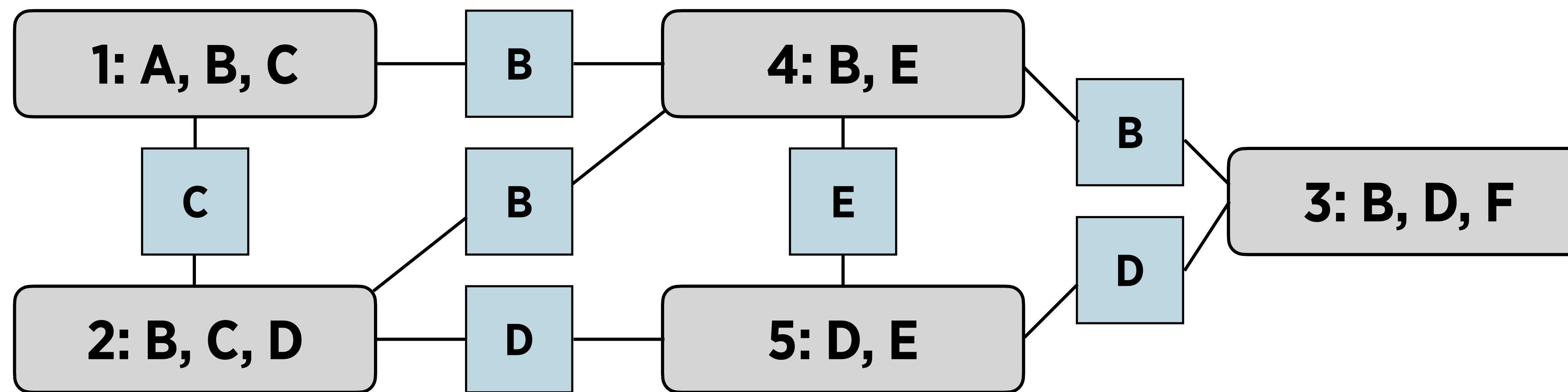


# Different cluster graph

$\phi_1(A, B, C), \phi_2(B, C), \phi_3(B, D), \phi_4(D, E), \phi_5(B, E), \phi_6(B, D), \phi_7(B, D, F)$

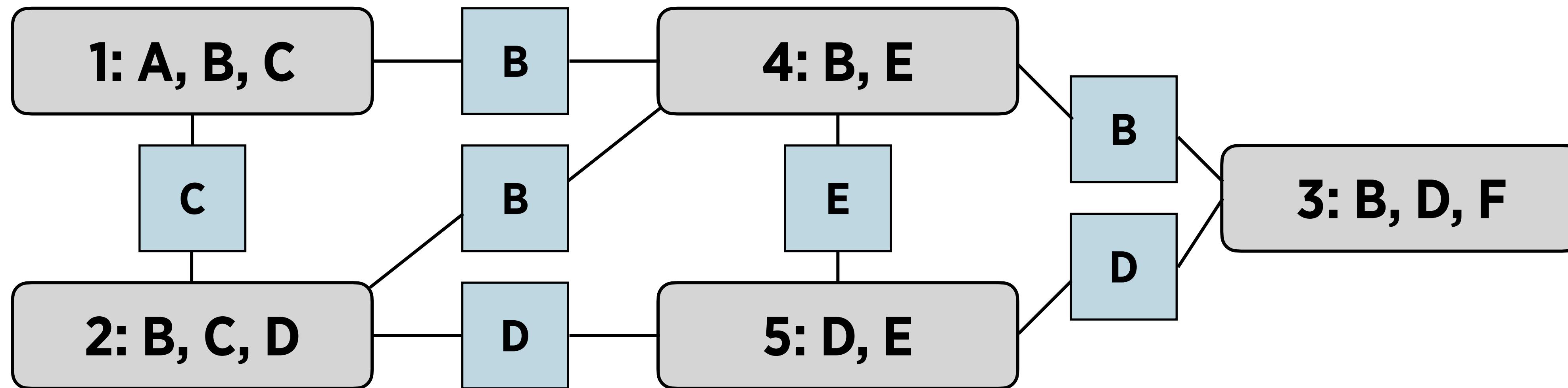


# Message passing



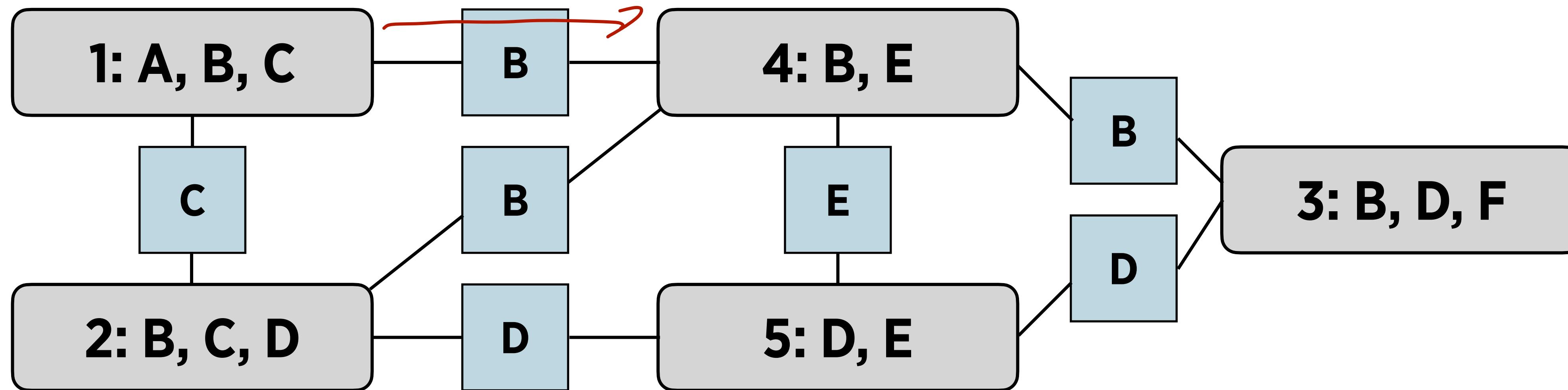
# Message passing

$$\delta_{1 \rightarrow 4}(B) = \sum_{A,C} \psi_1(A, B, C) \delta_{2 \rightarrow 1}(C)$$



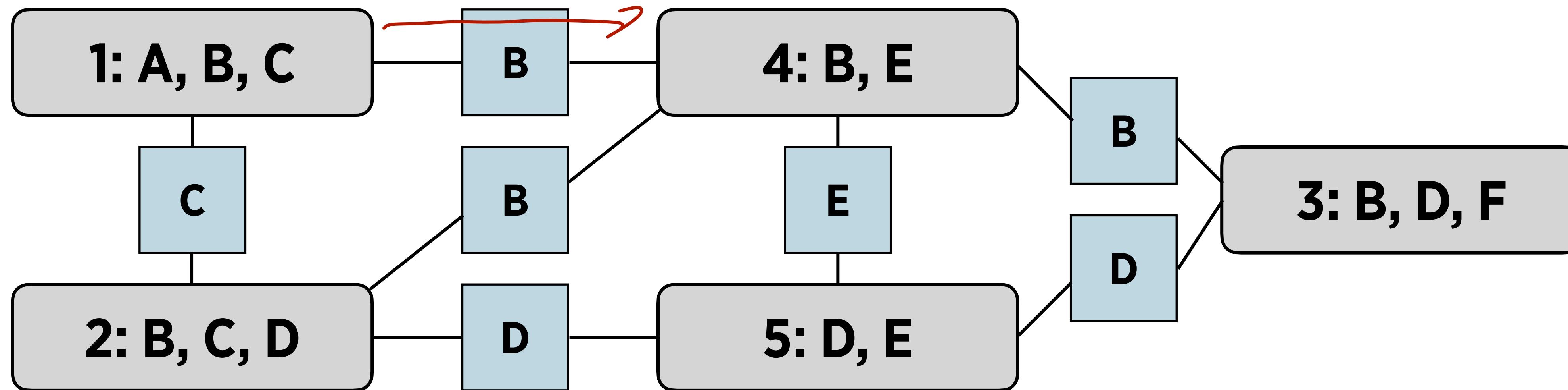
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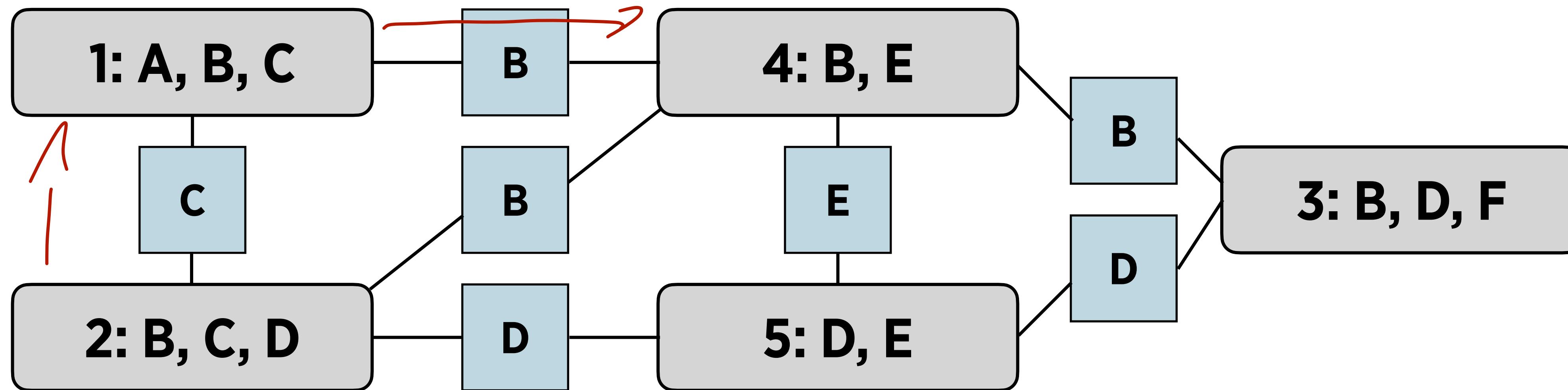
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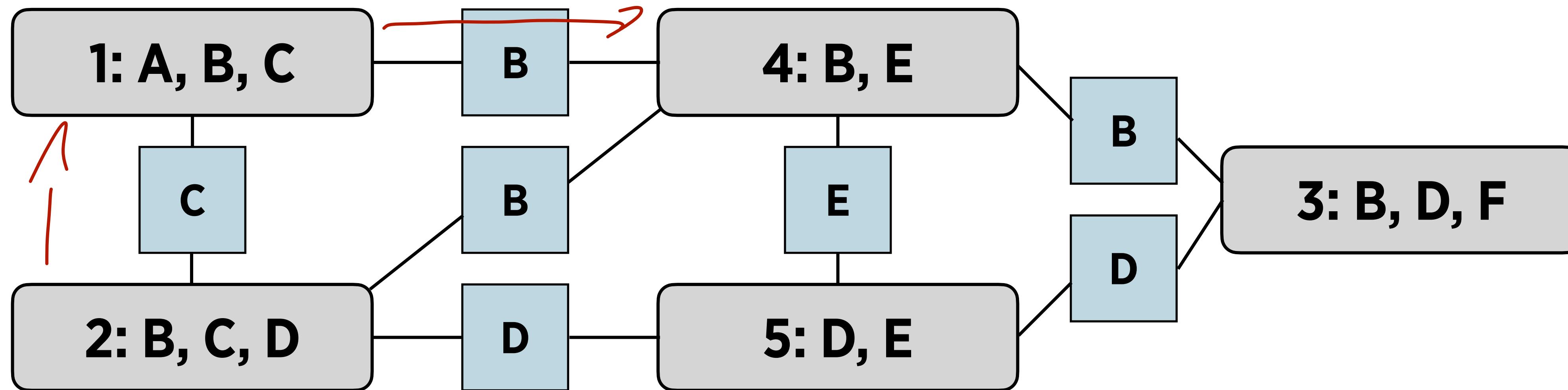
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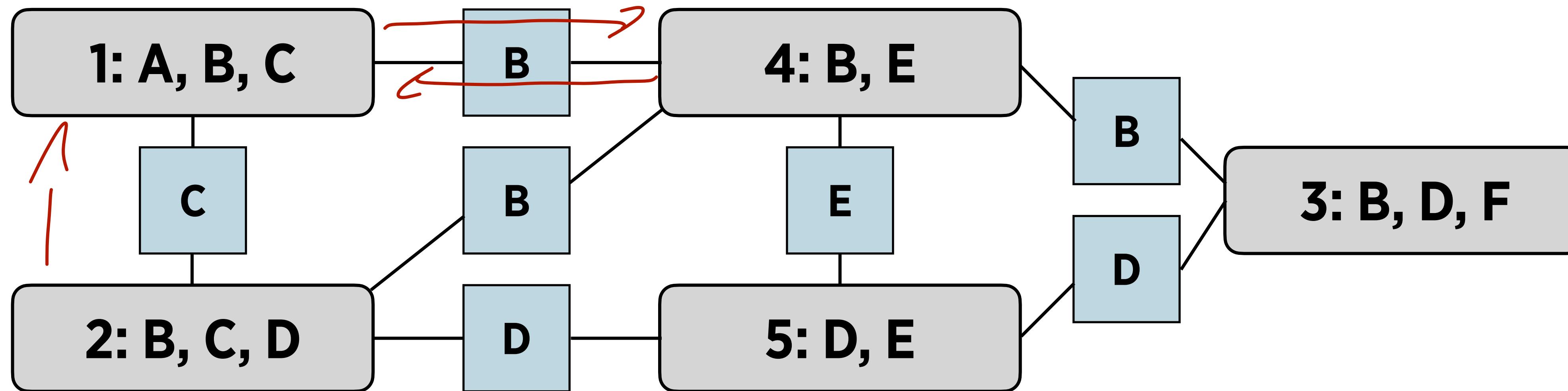
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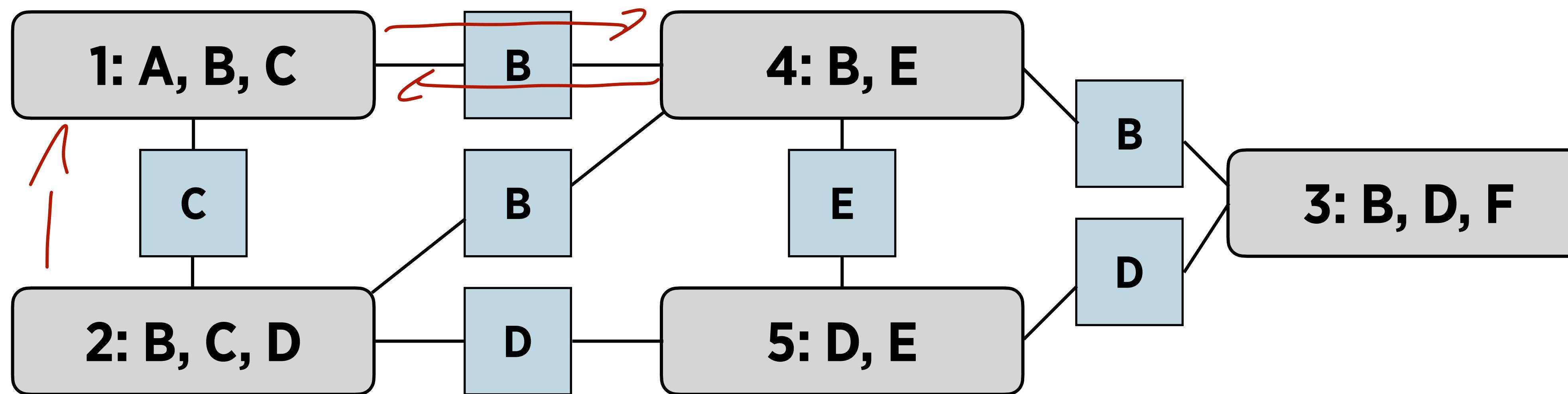
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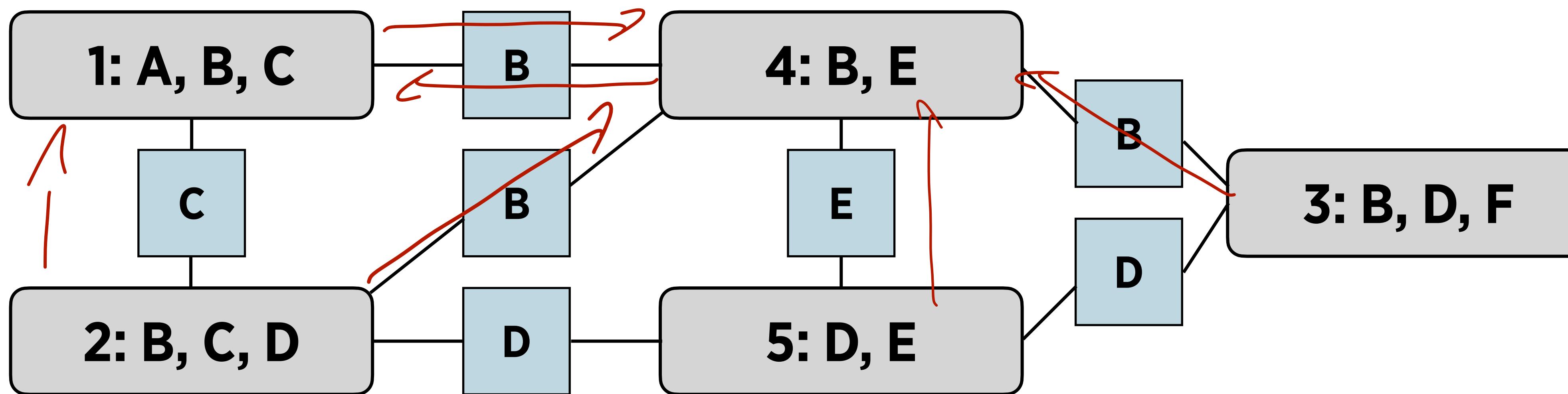
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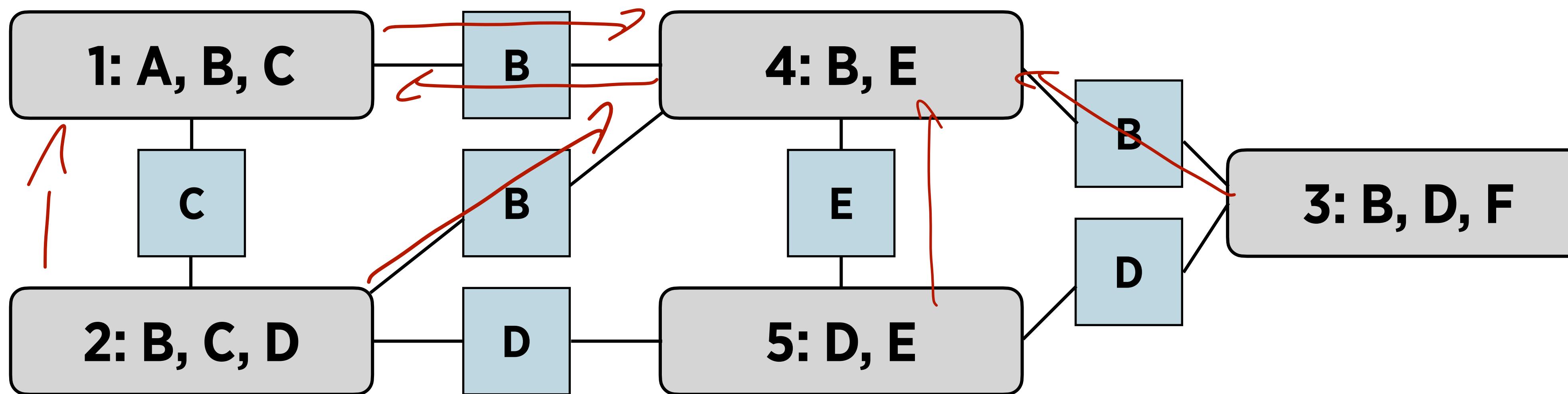
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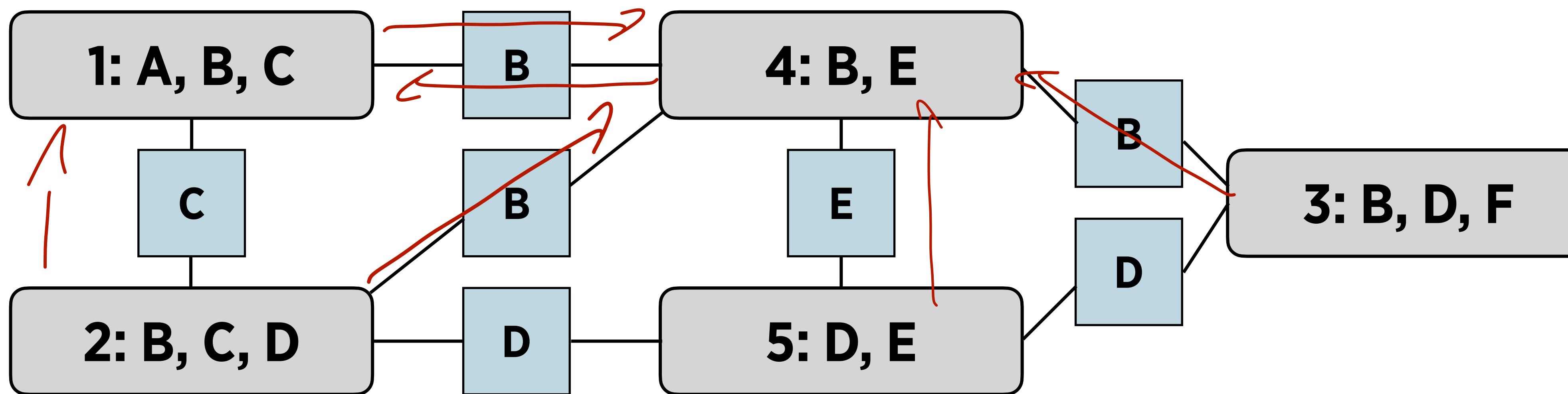


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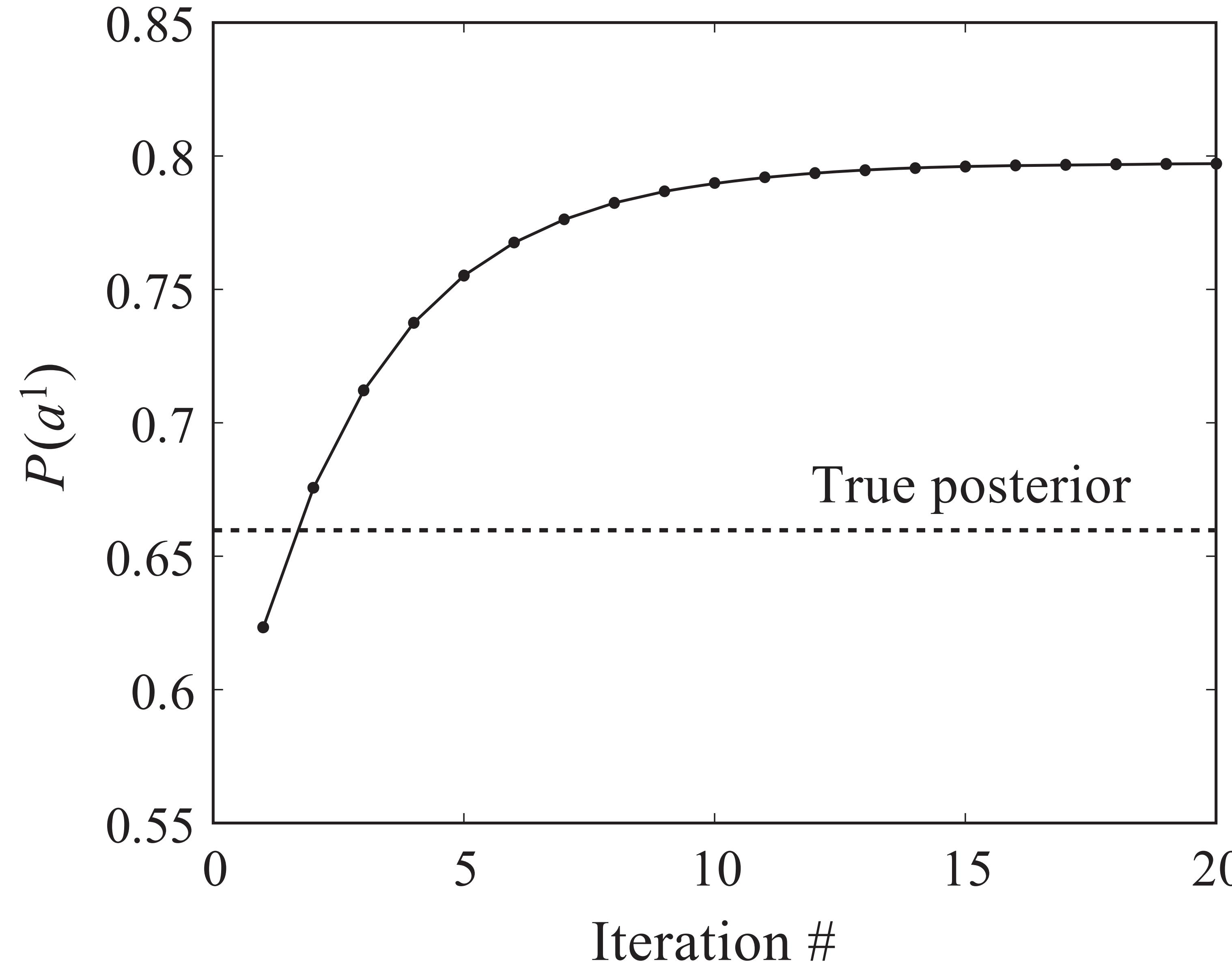
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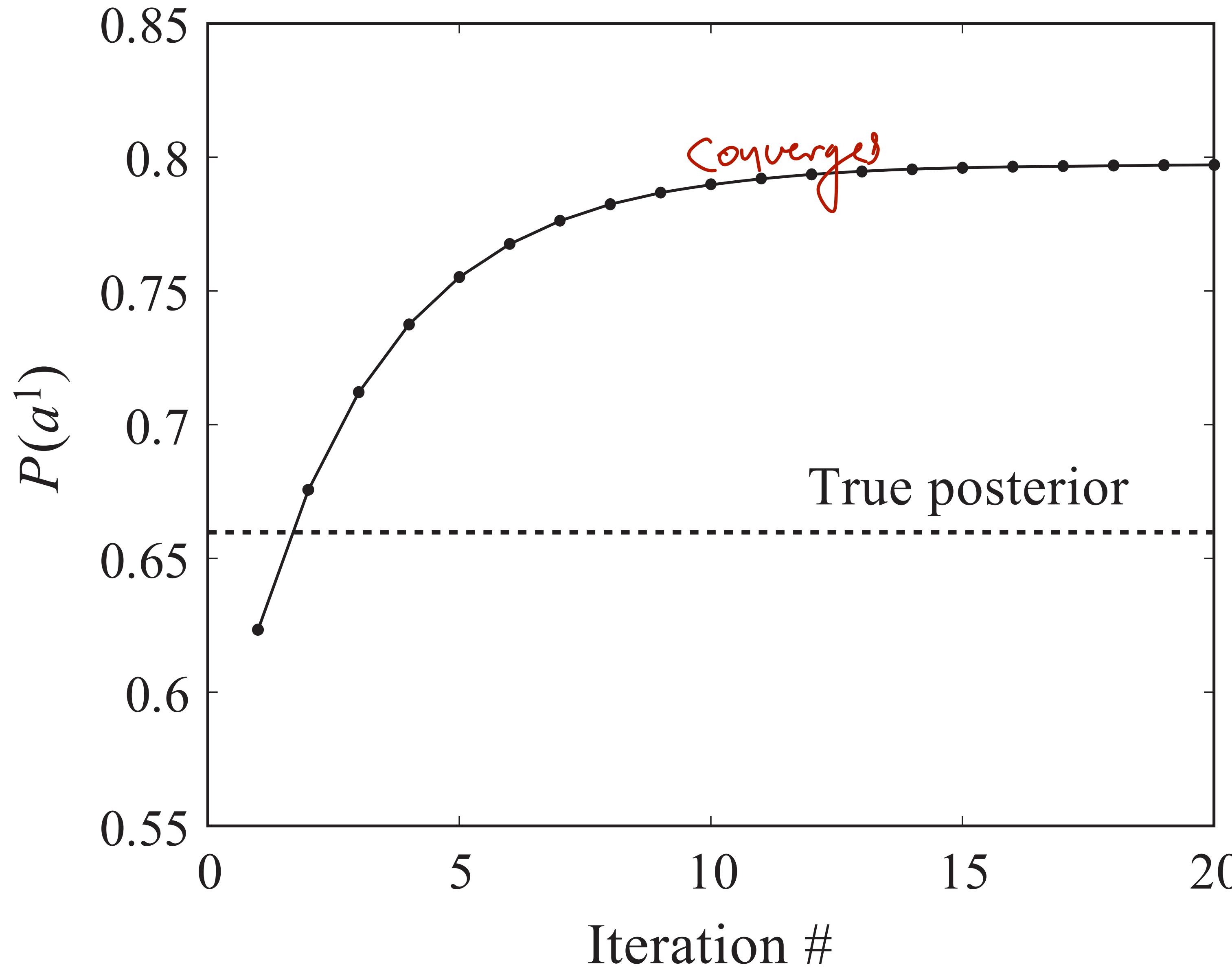
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e.g. round robin

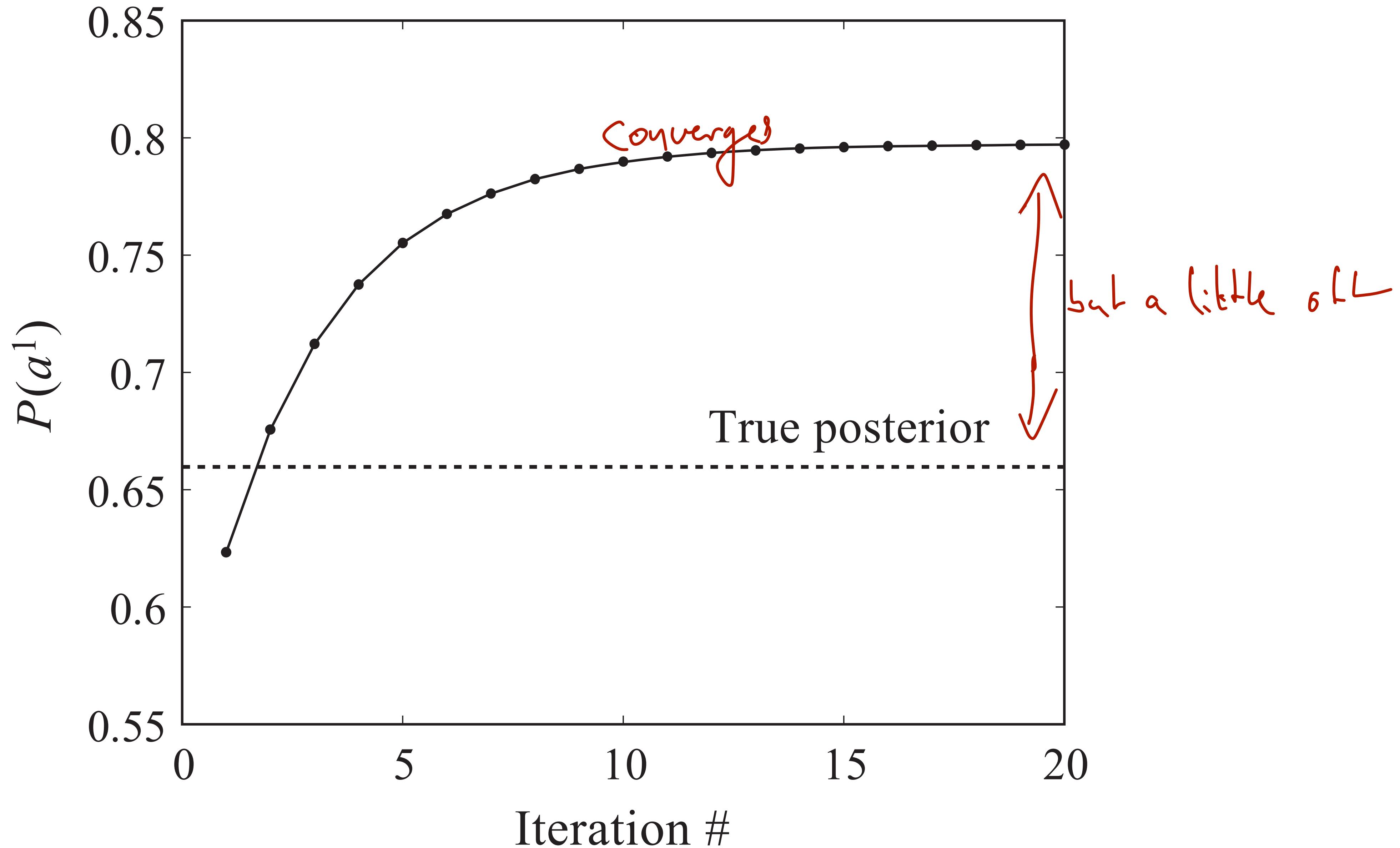
# Belief propagation run



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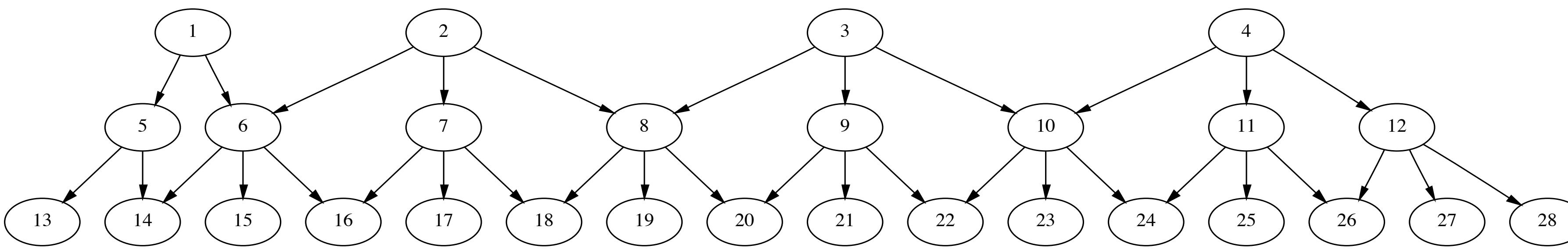


Figure 1: The structure of the PYRAMID network. All nodes are binary and observations appear only on the bottom layer. Such networks occur often in image analysis where the bottom layer would correspond to pixels.

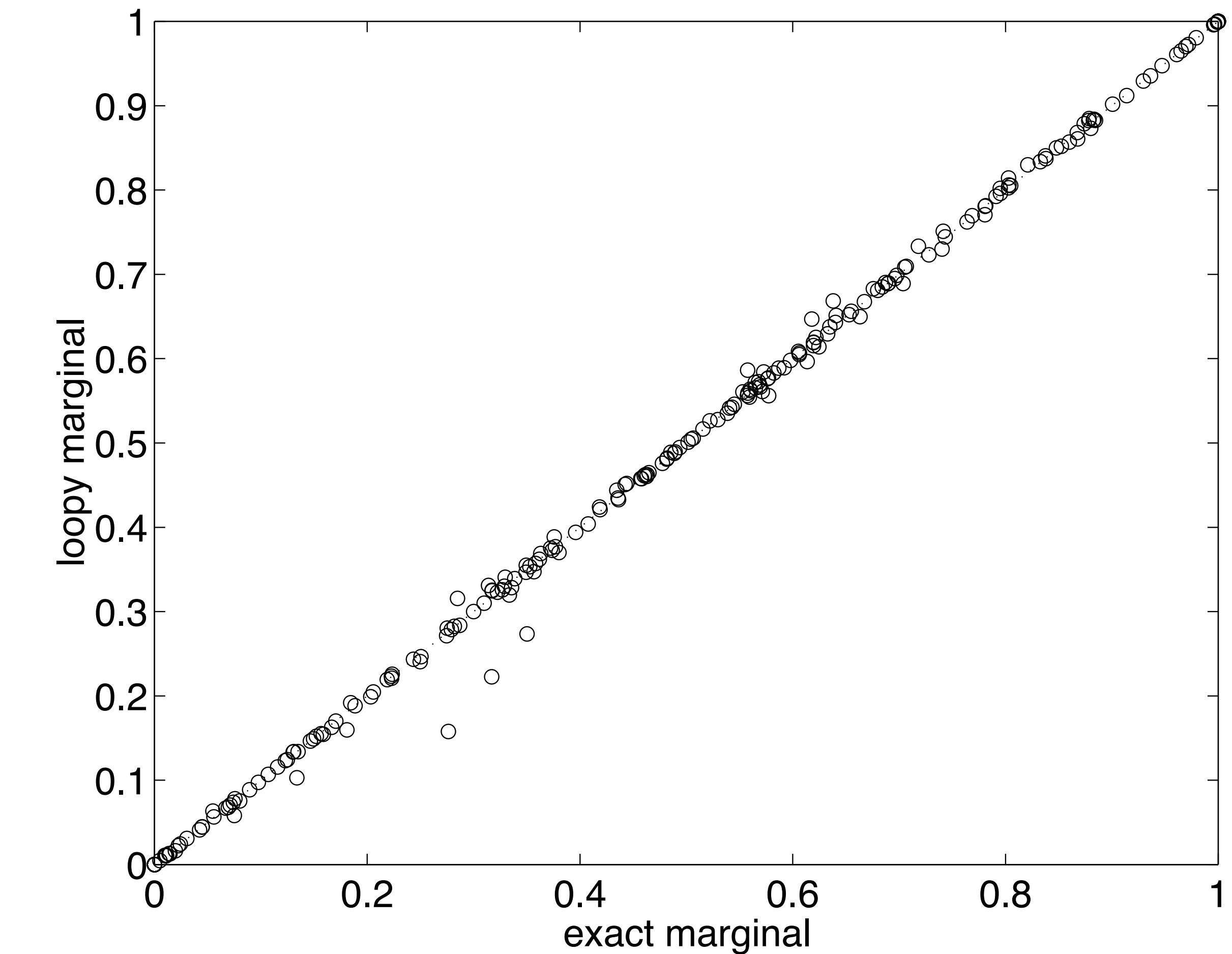
Murphy, Weiss, Jordan, UAI'99

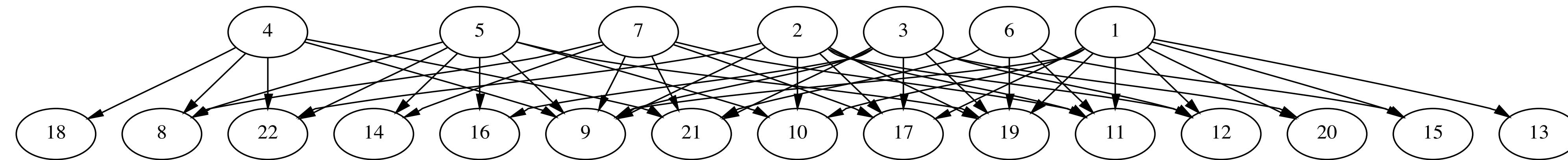
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## Loopy Belief Propagation for Approximate Inference: An Empirical Study

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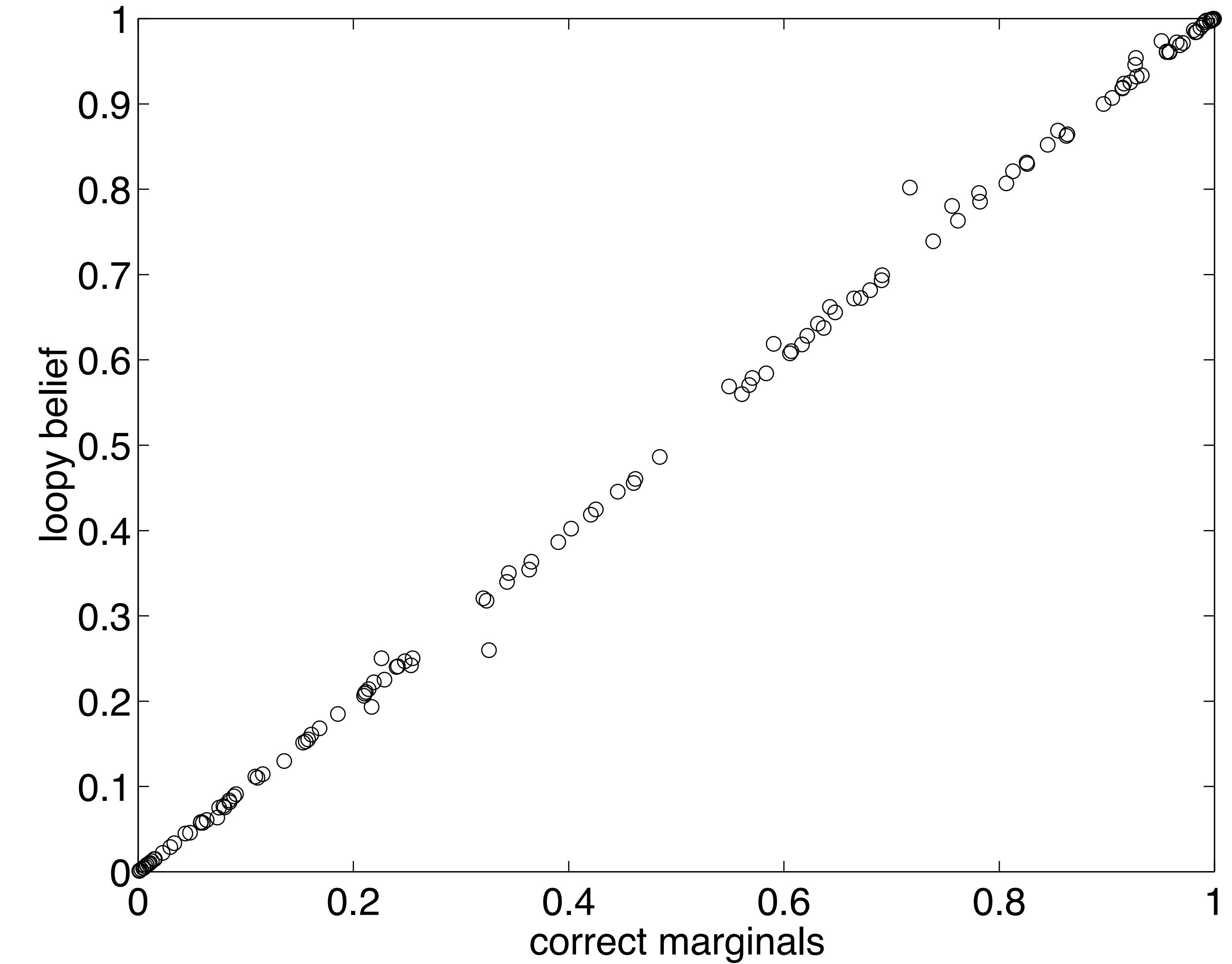
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- Algorithm may not converge
- The resulting beliefs are pseudo-marginals (not necessarily exact)
- Nevertheless, very useful in practice

# Cluster Graph Properties

# Cluster Graphs

- Undirected graph such that:
  - Nodes are clusters  $C_i \subseteq \{X_1, \dots, X_n\}$
  - Edge between  $C_i$  and  $C_j$  associated with sepset  $S_{i,j} \subseteq C_i \cap C_j$ 
    - Separation set: variables on both sides are separated by variables in  $S$

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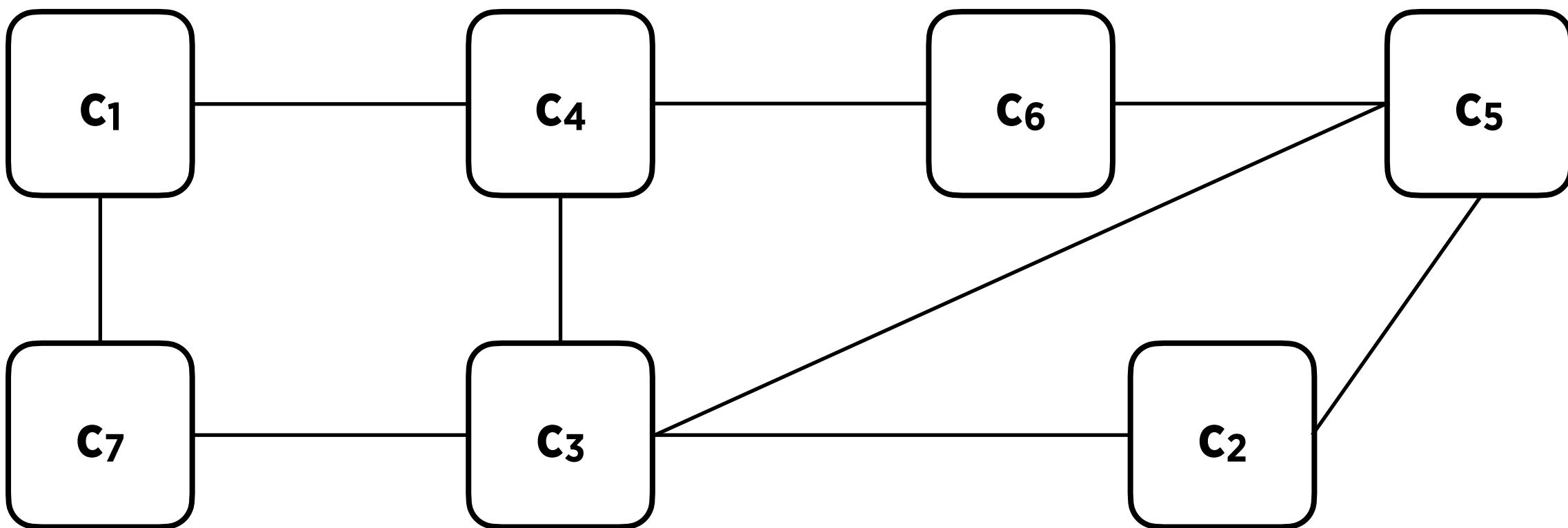
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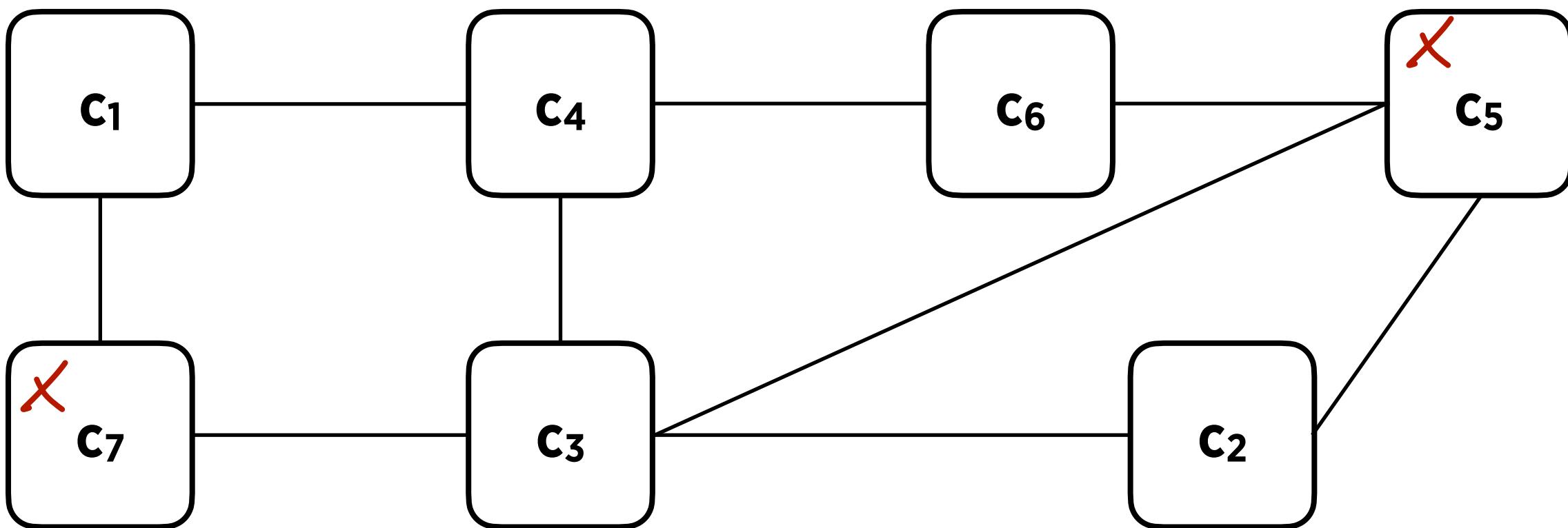
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- For each pair of clusters  $C_i, C_j$ , and variable  $X \in C_i \cap C_j$  there exists a unique path between  $C_i$  and  $C_j$  for which all clusters and sepsets contain  $X$



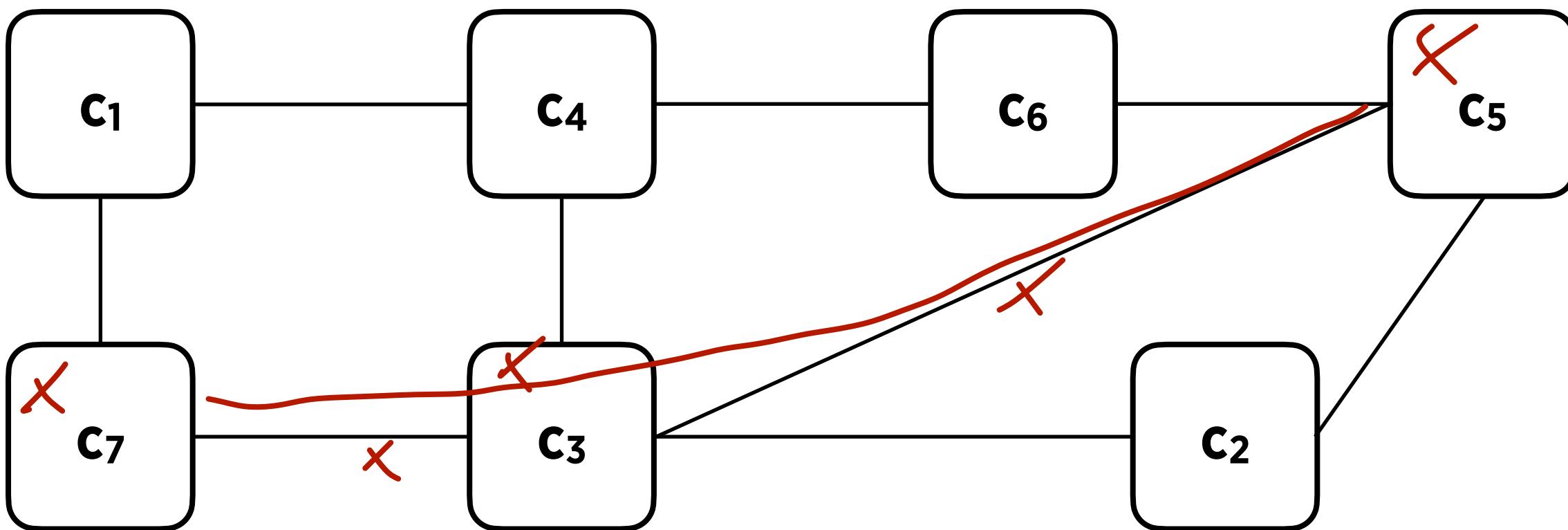
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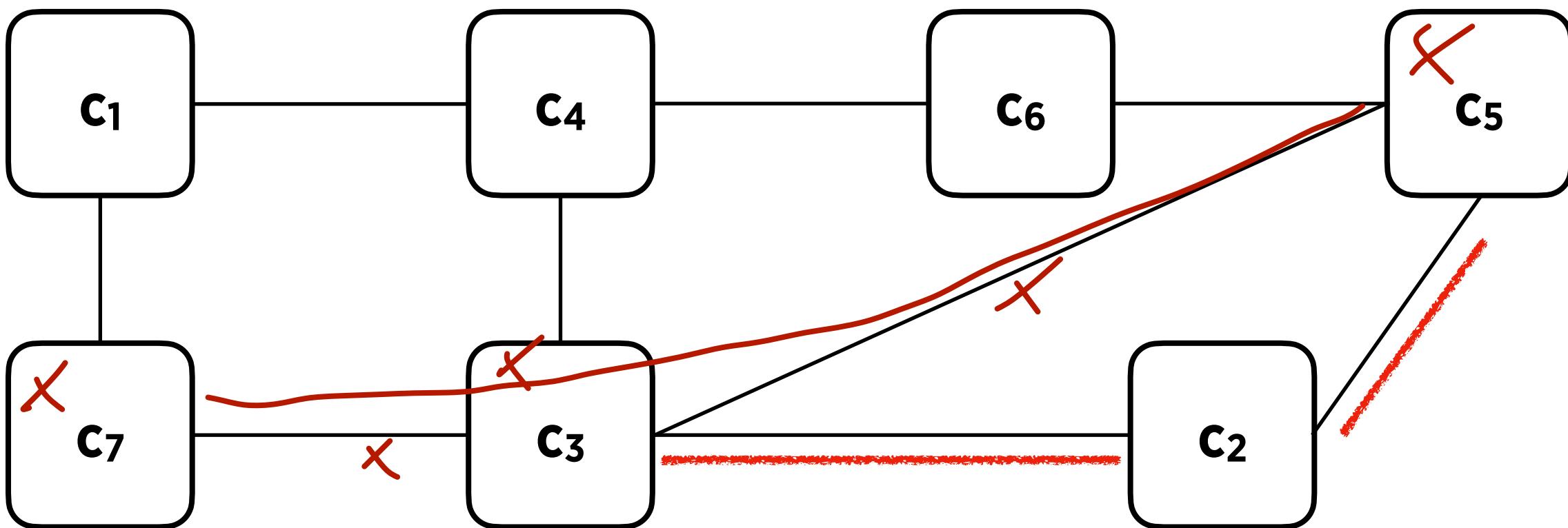
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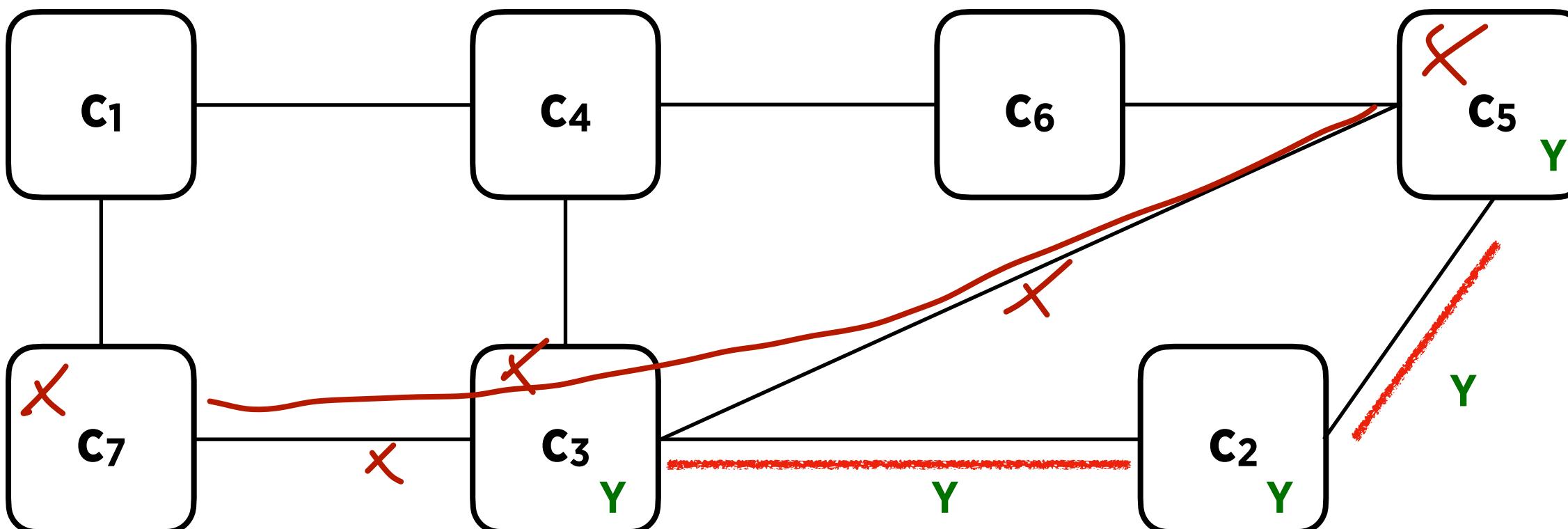
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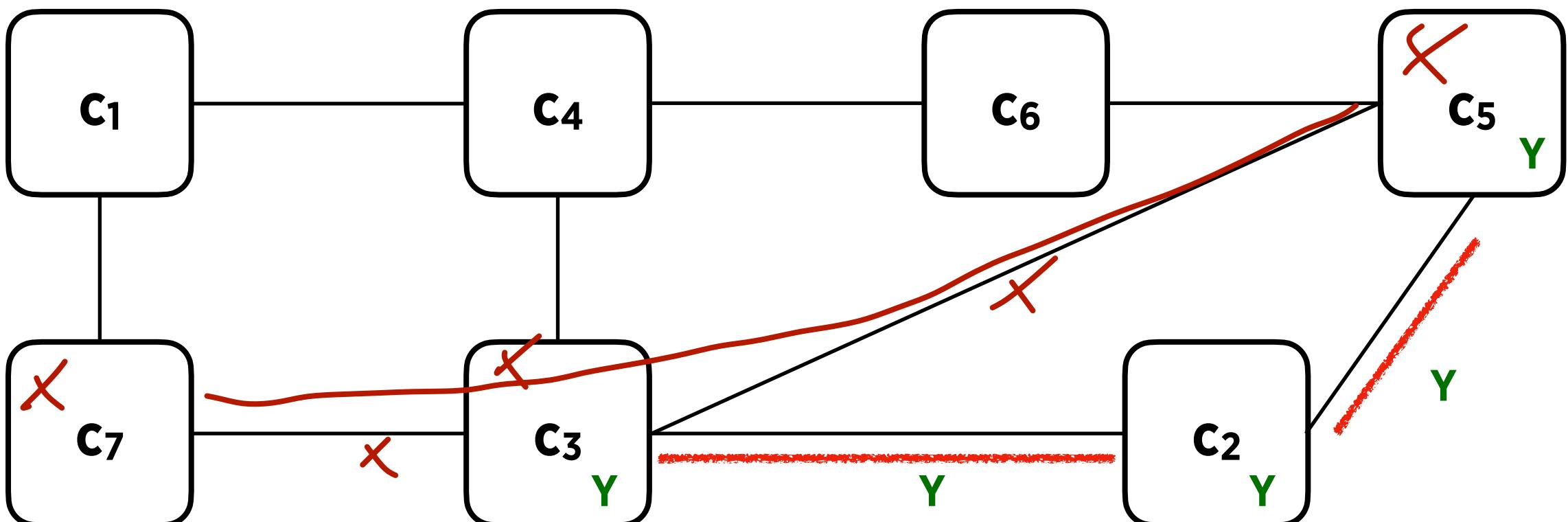
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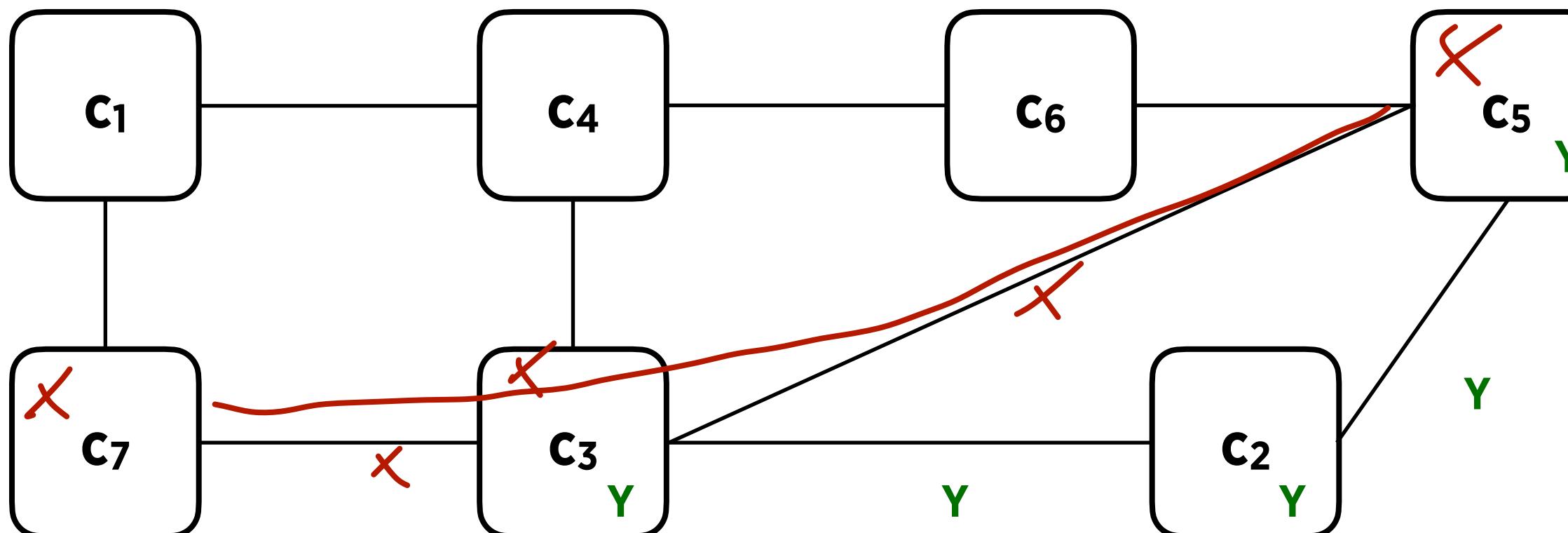
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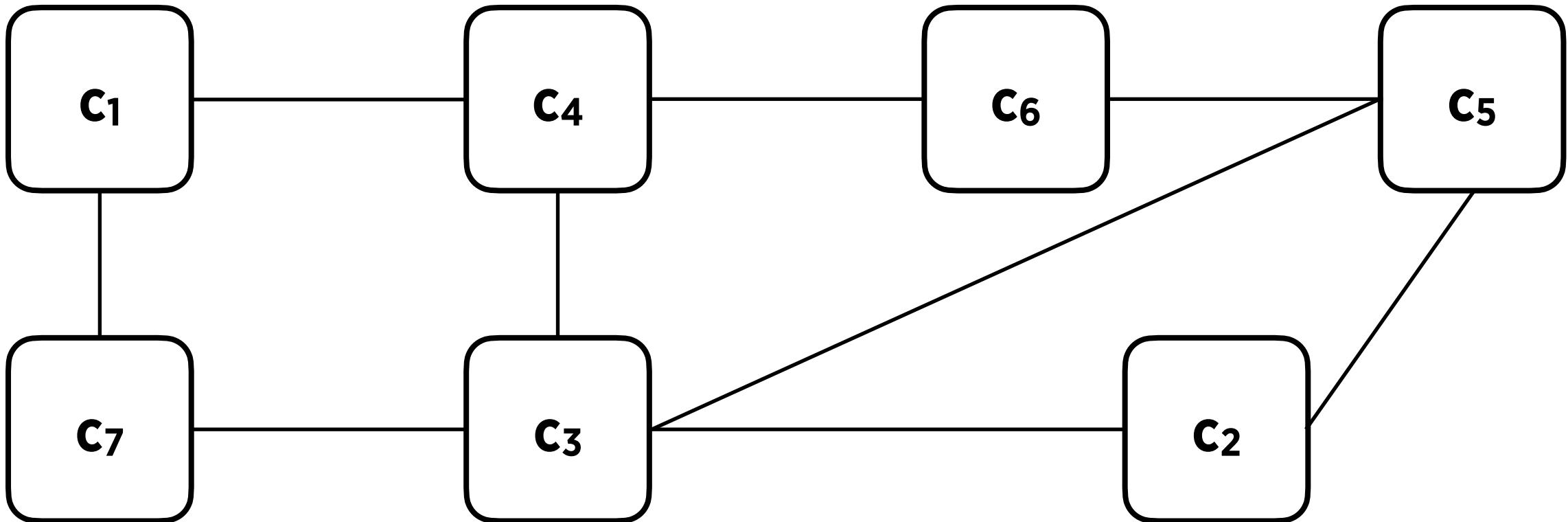
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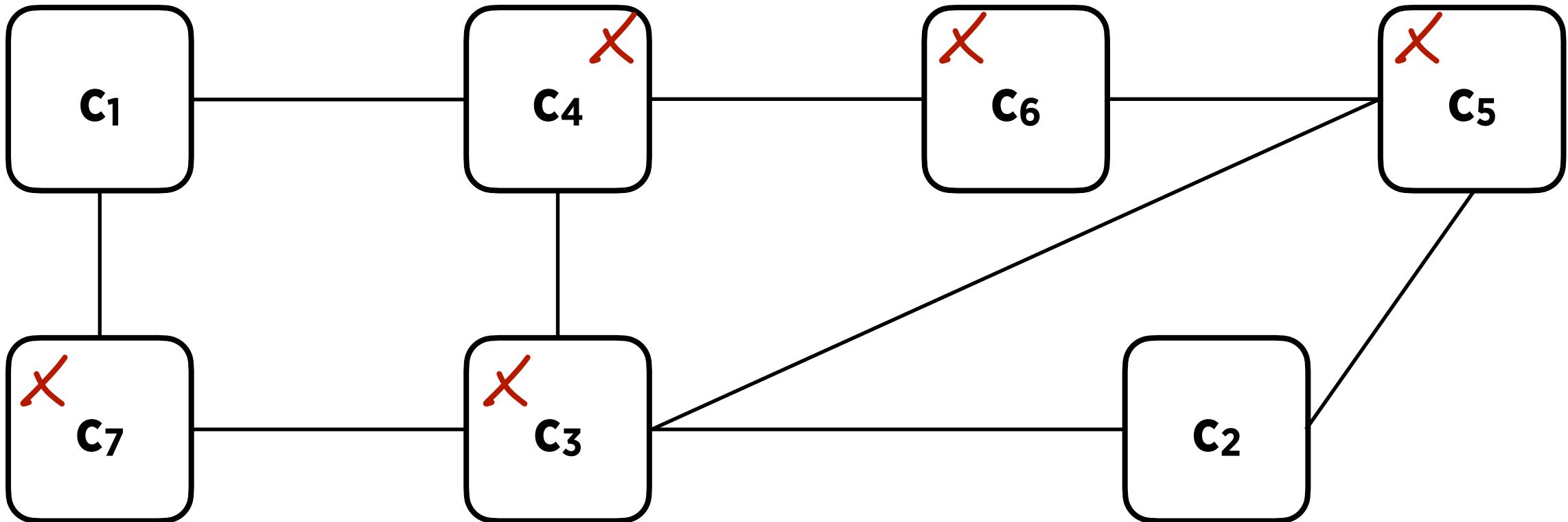
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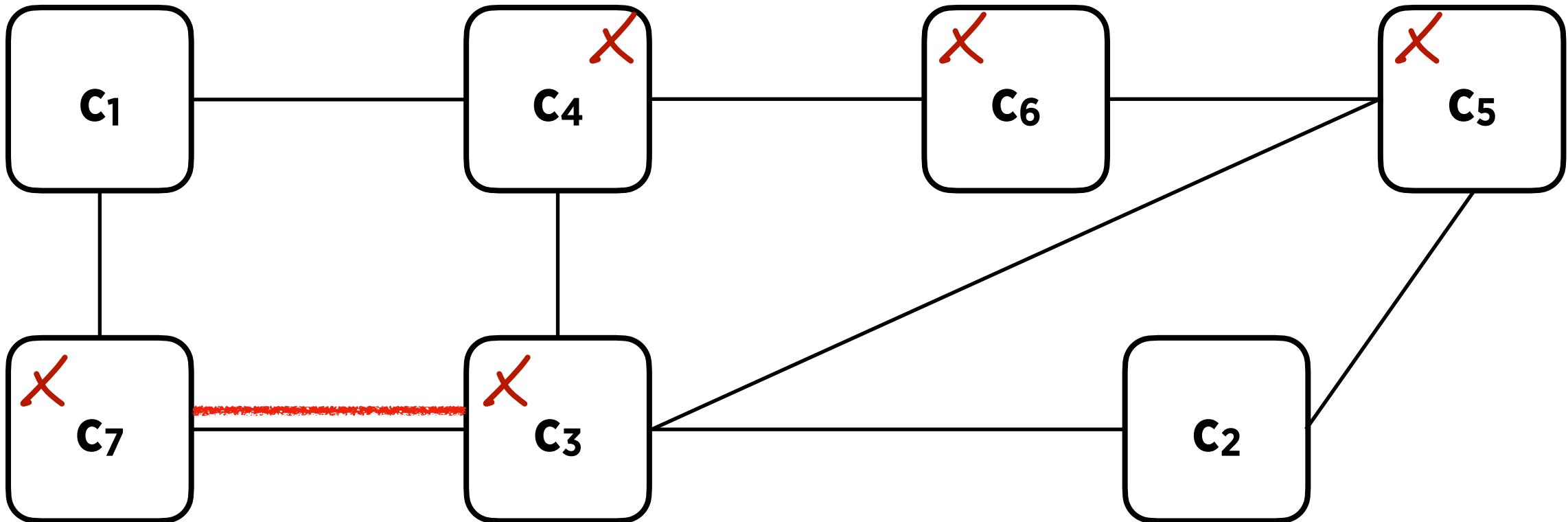
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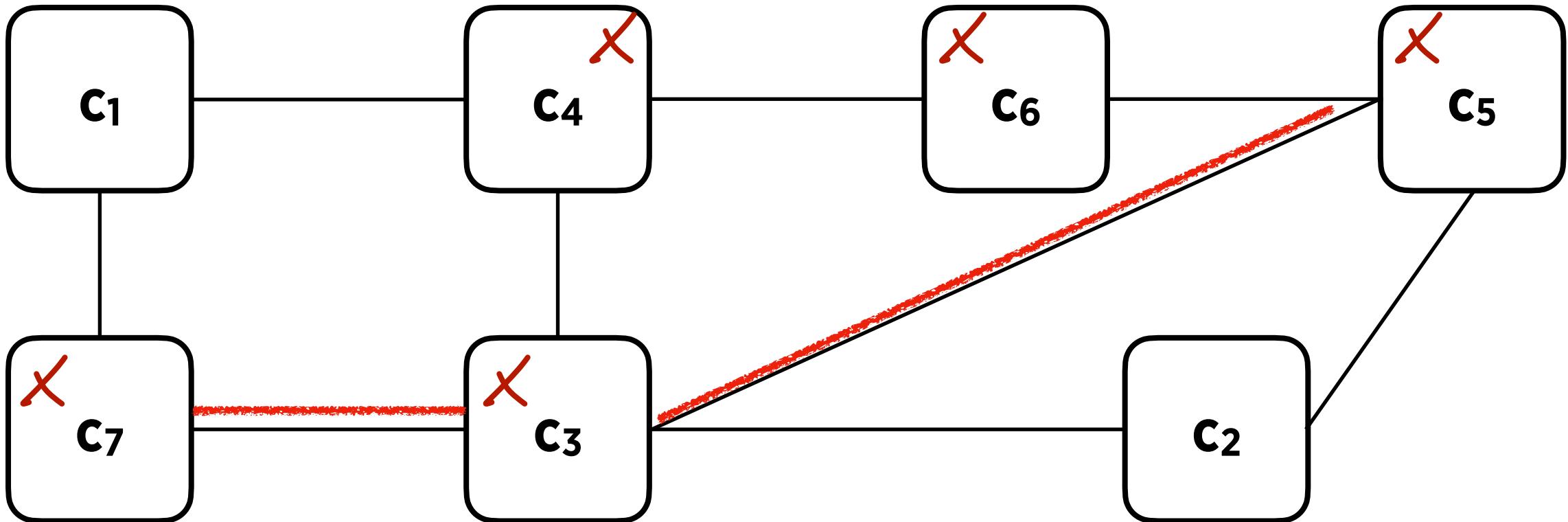
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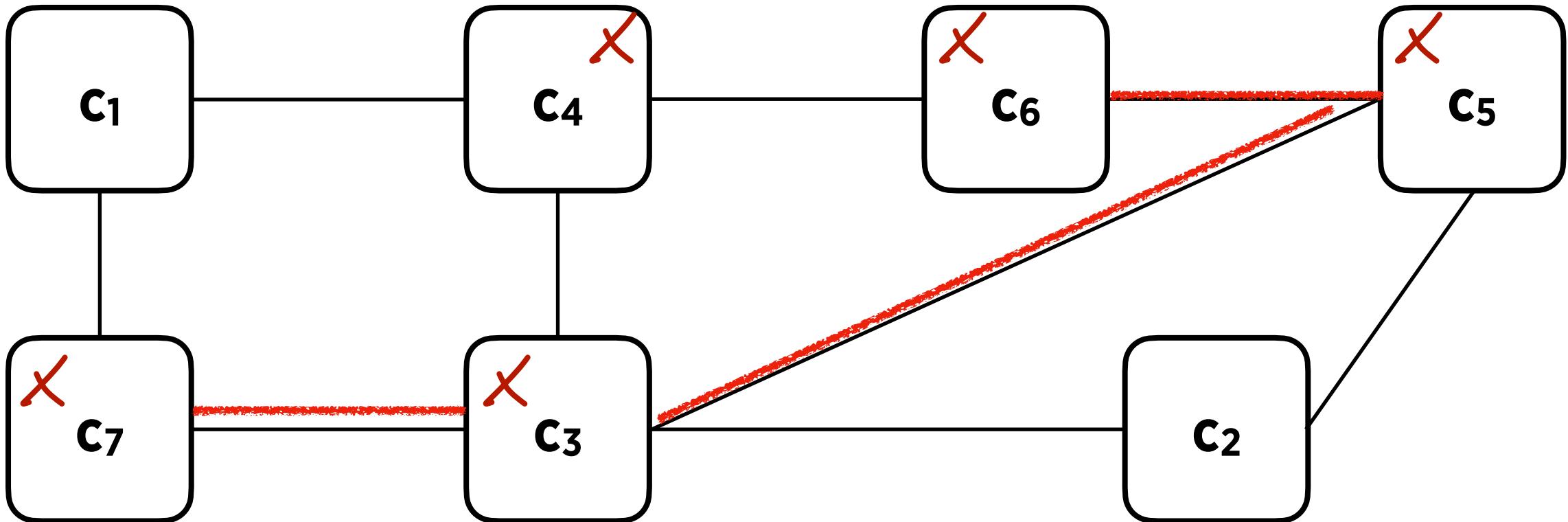
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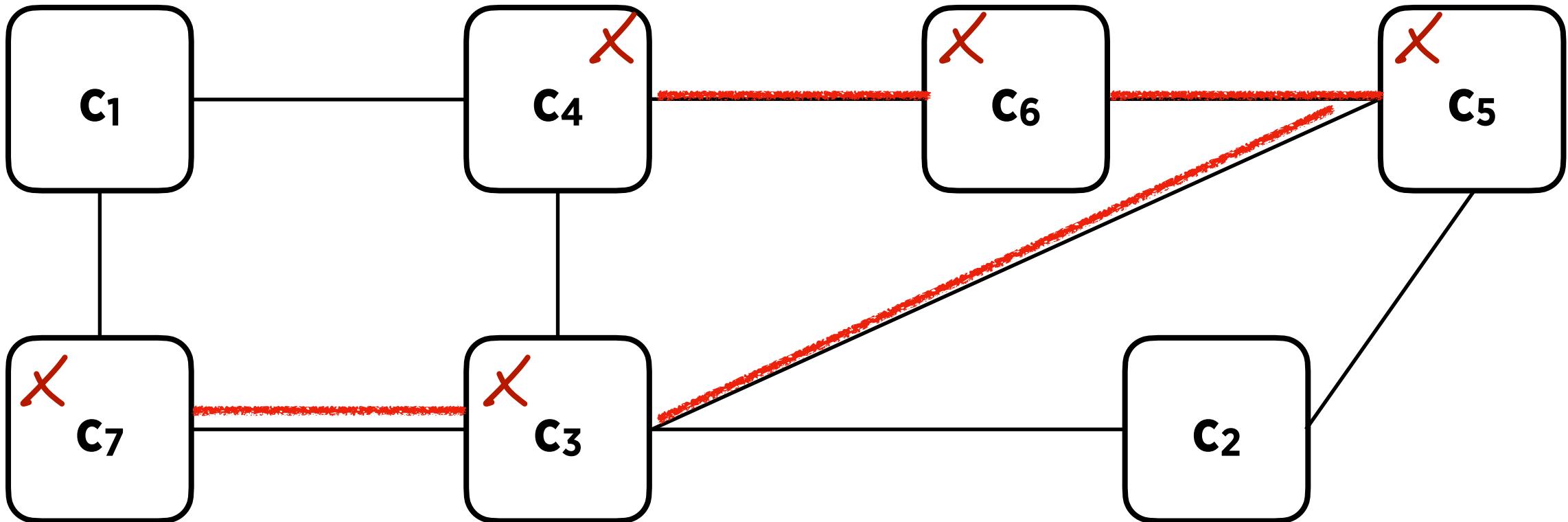
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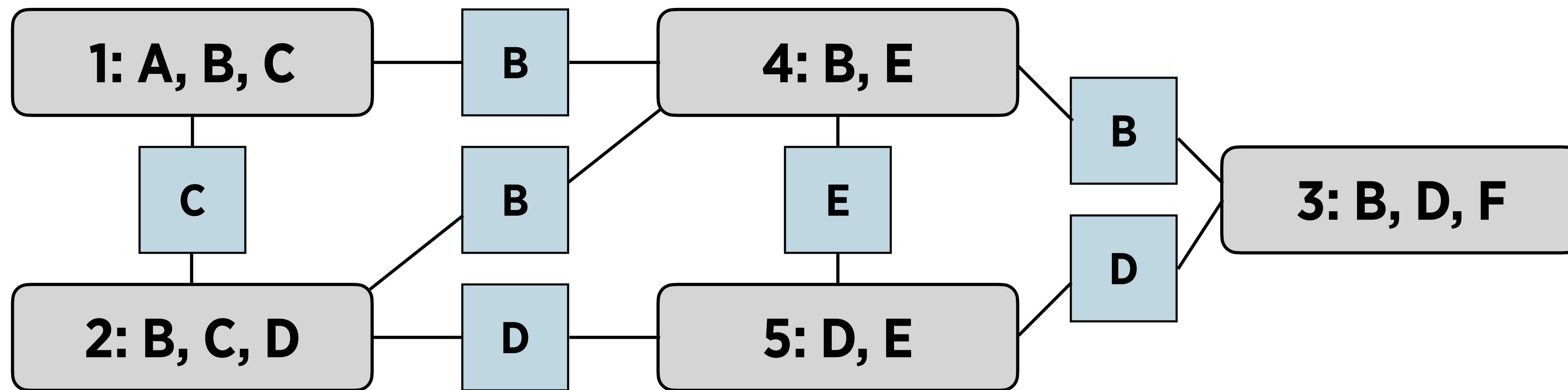
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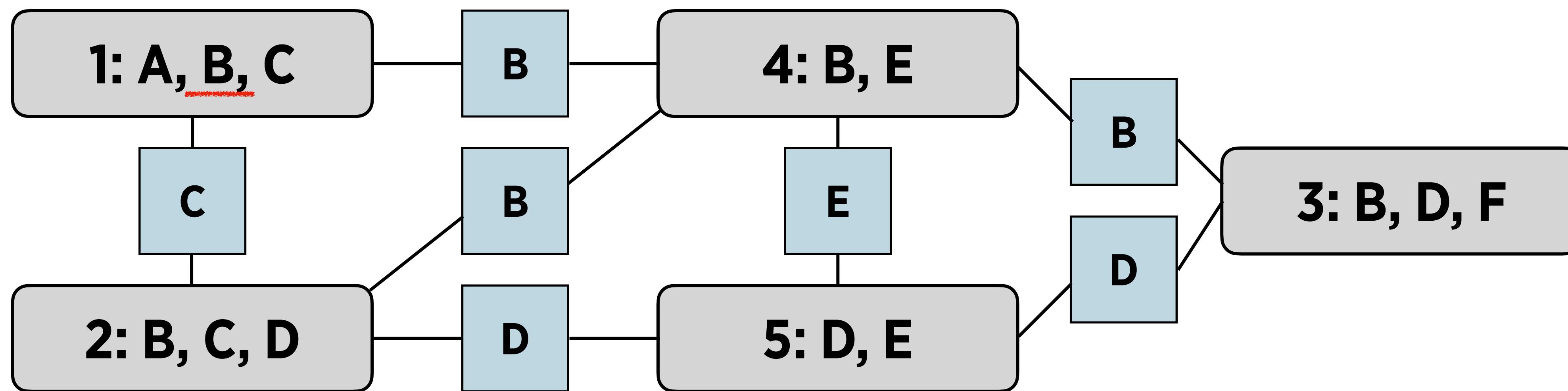
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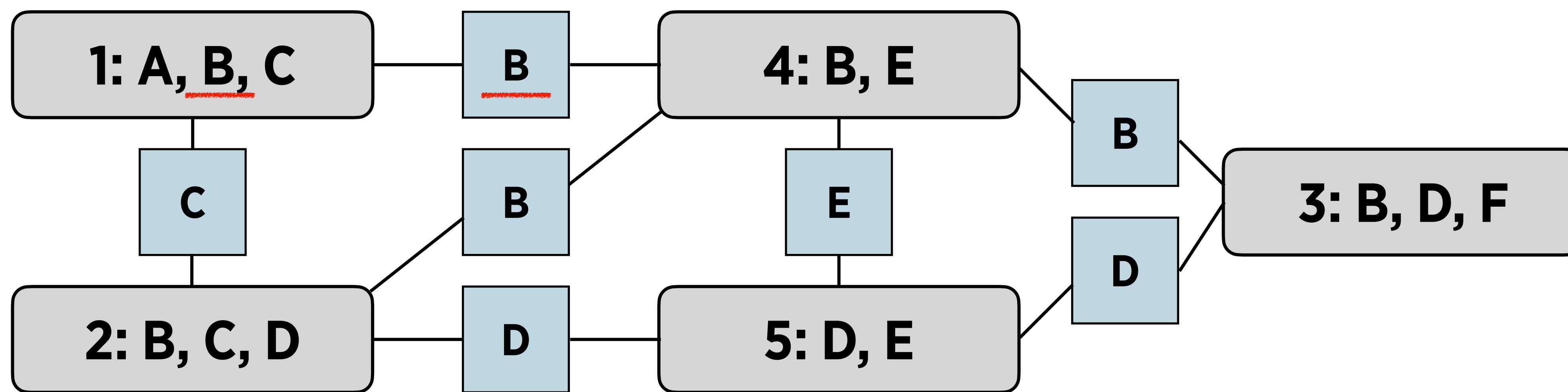
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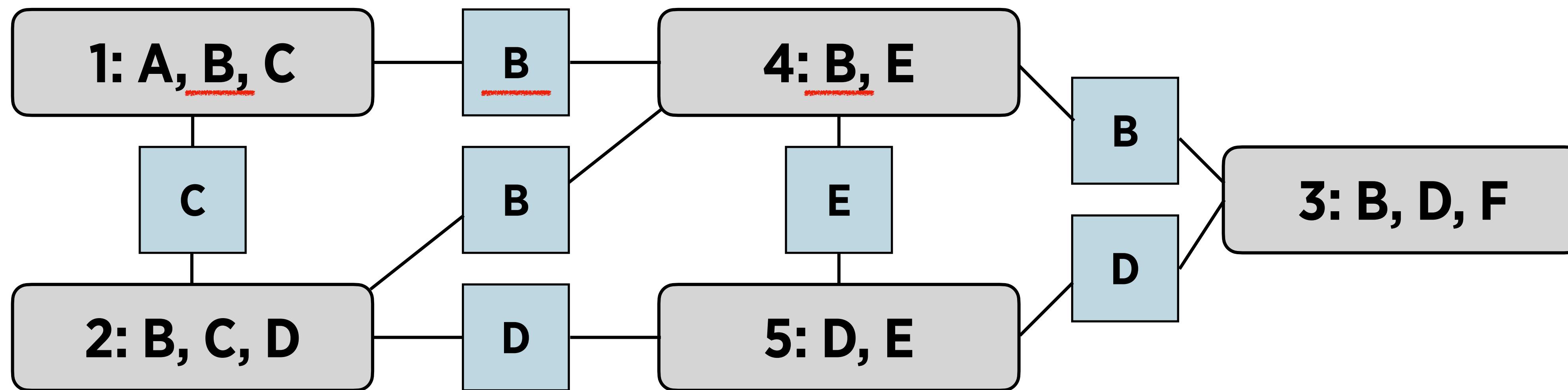
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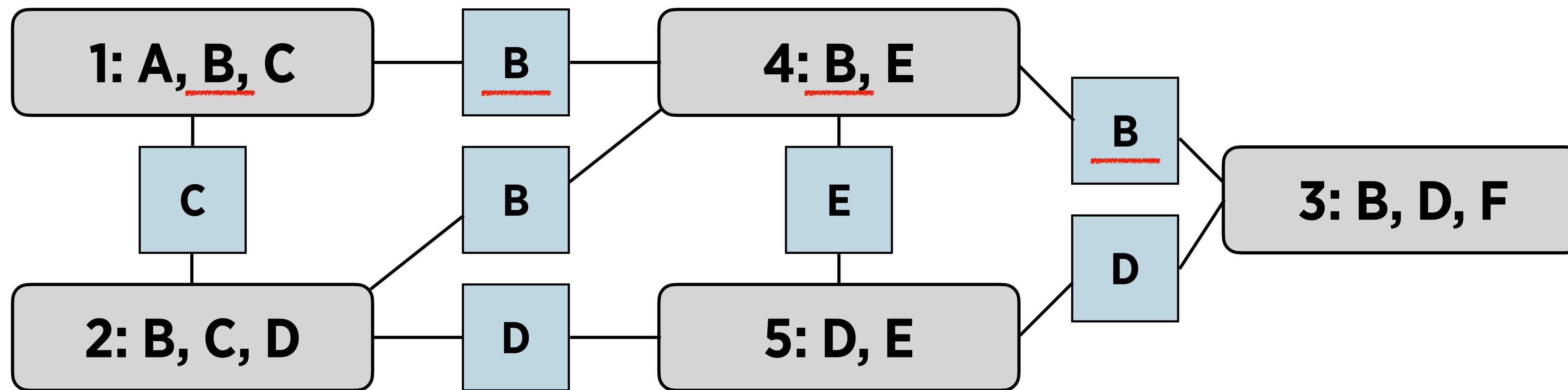
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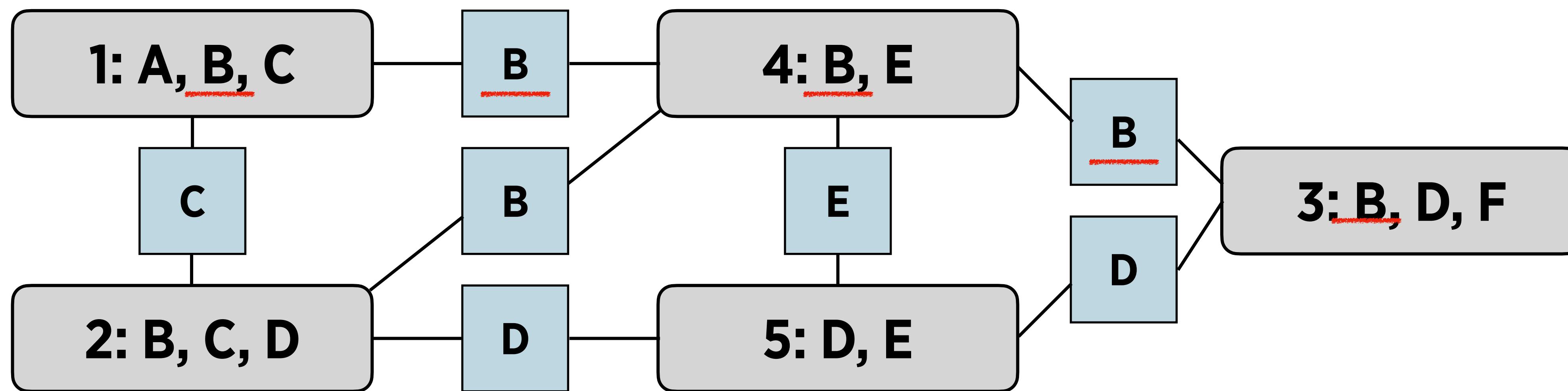
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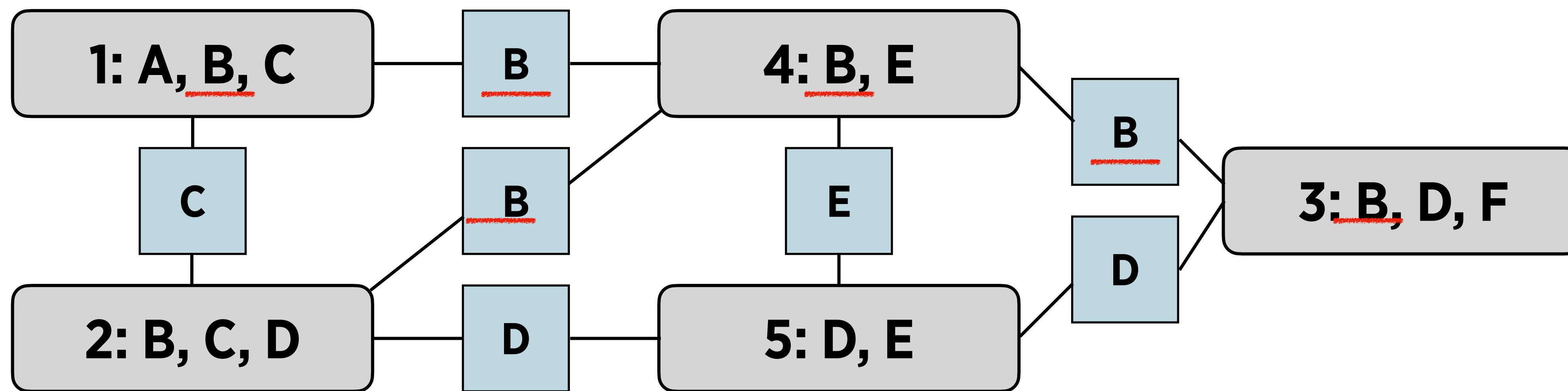
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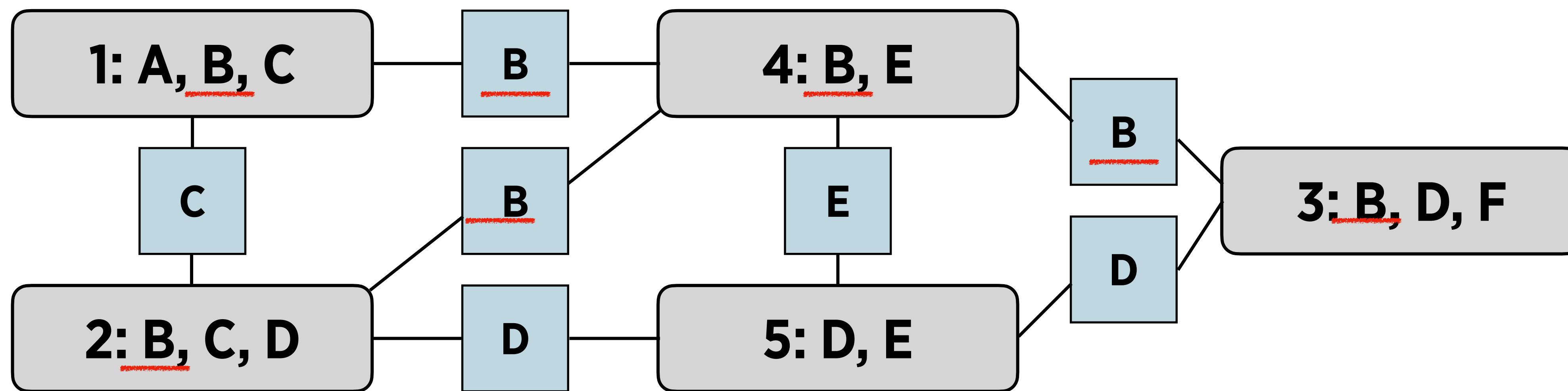
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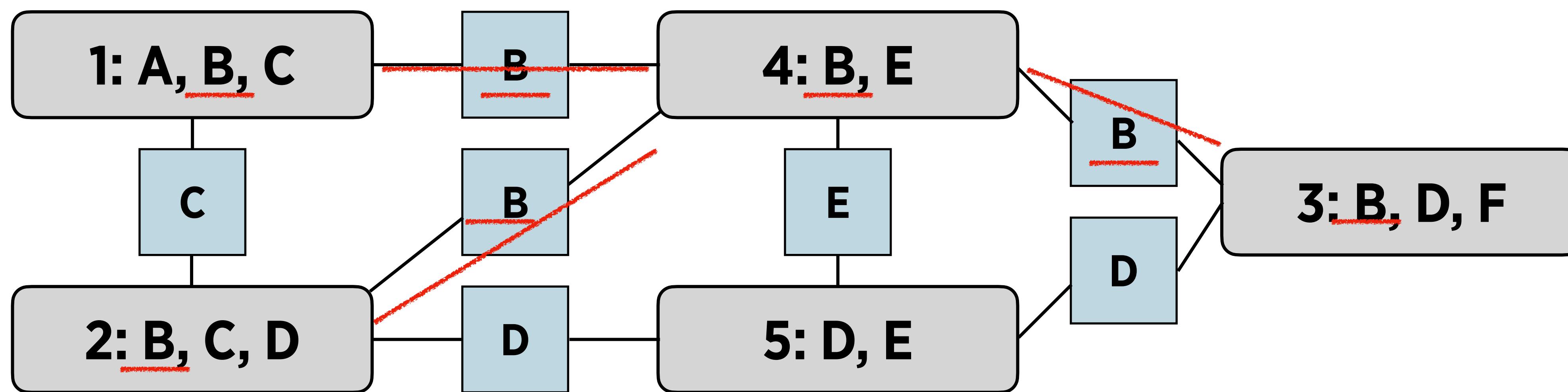
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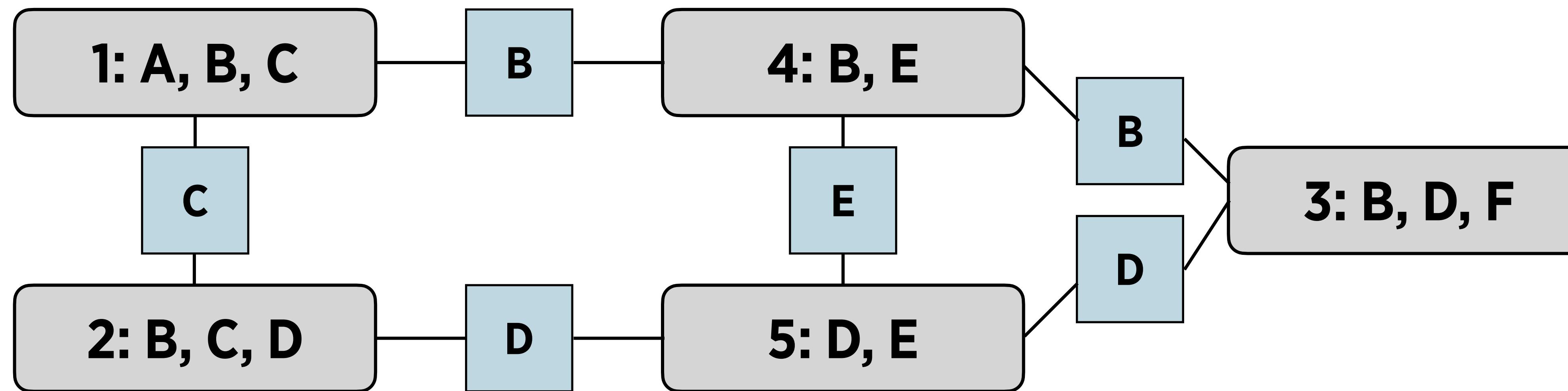


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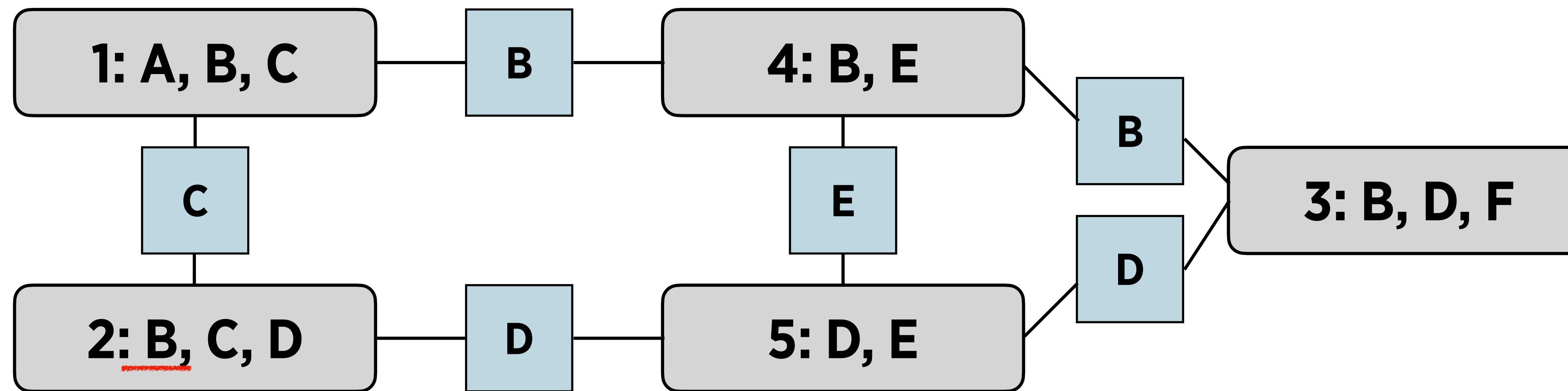
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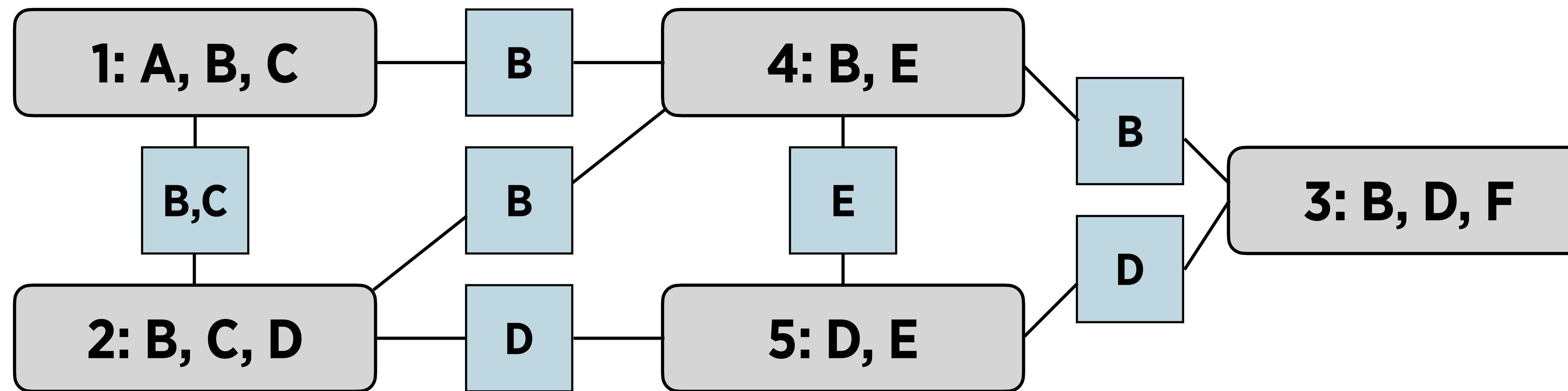
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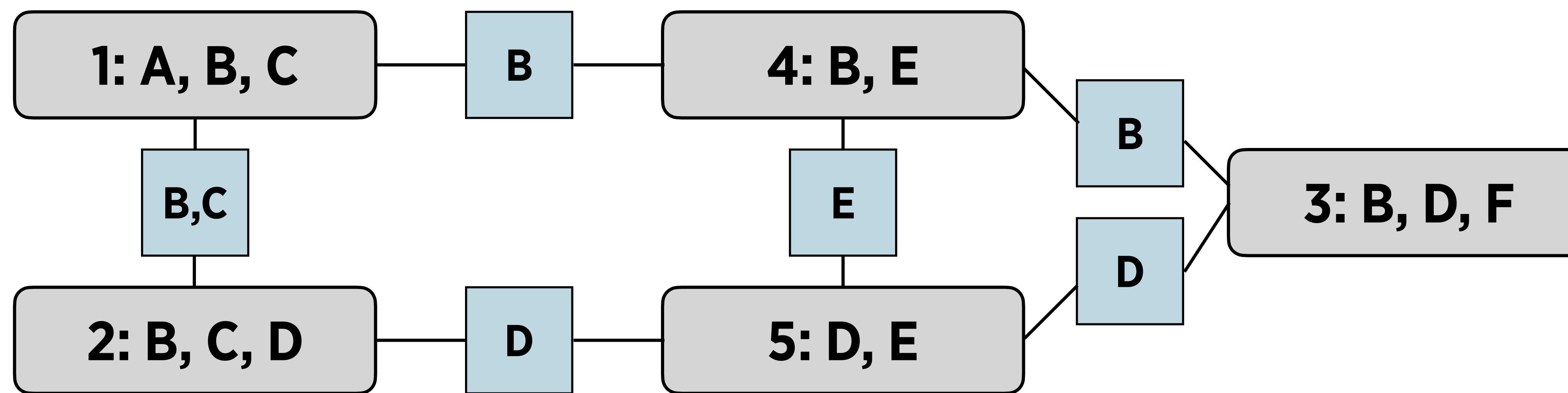
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# Illegal cluster graph (II)



# Alternative legal cluster graph



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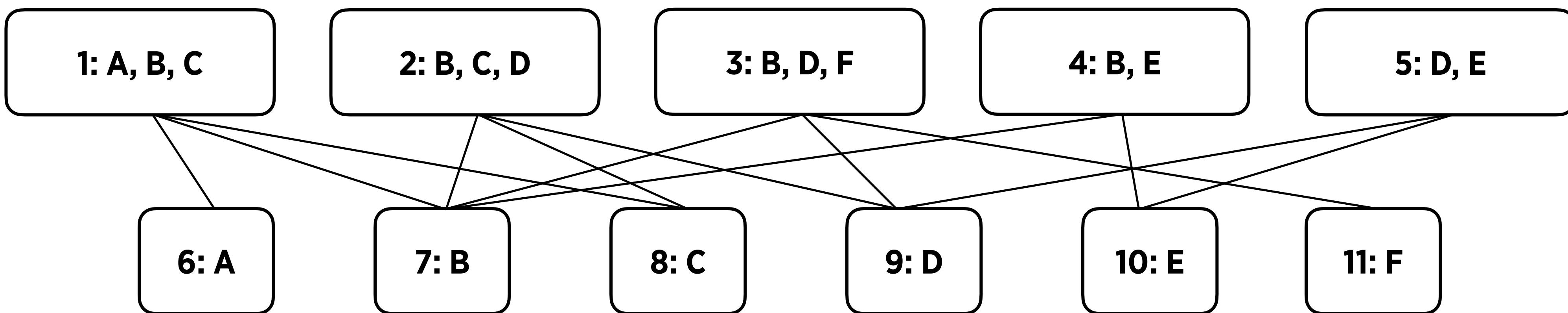
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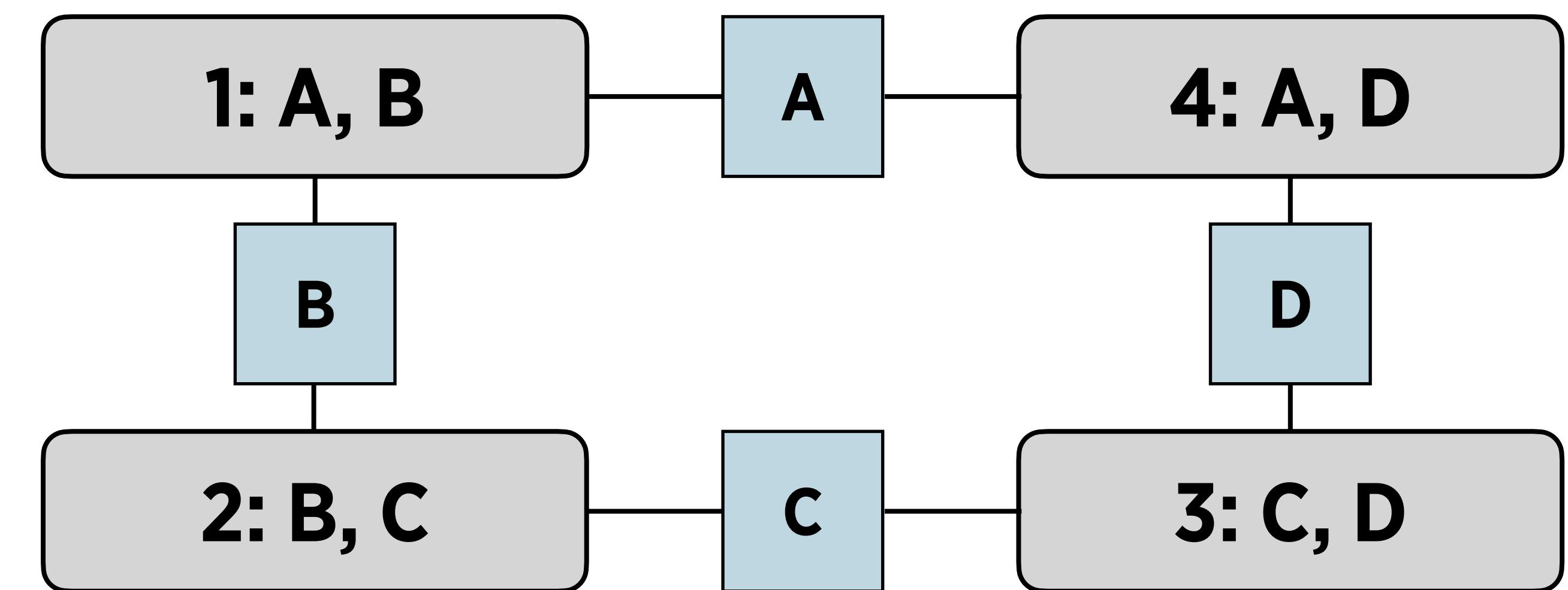
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- Bethe cluster graph is often first default
- Richer cluster graph structures can offer different tradeoffs wrt computational costs and preservation of dependencies

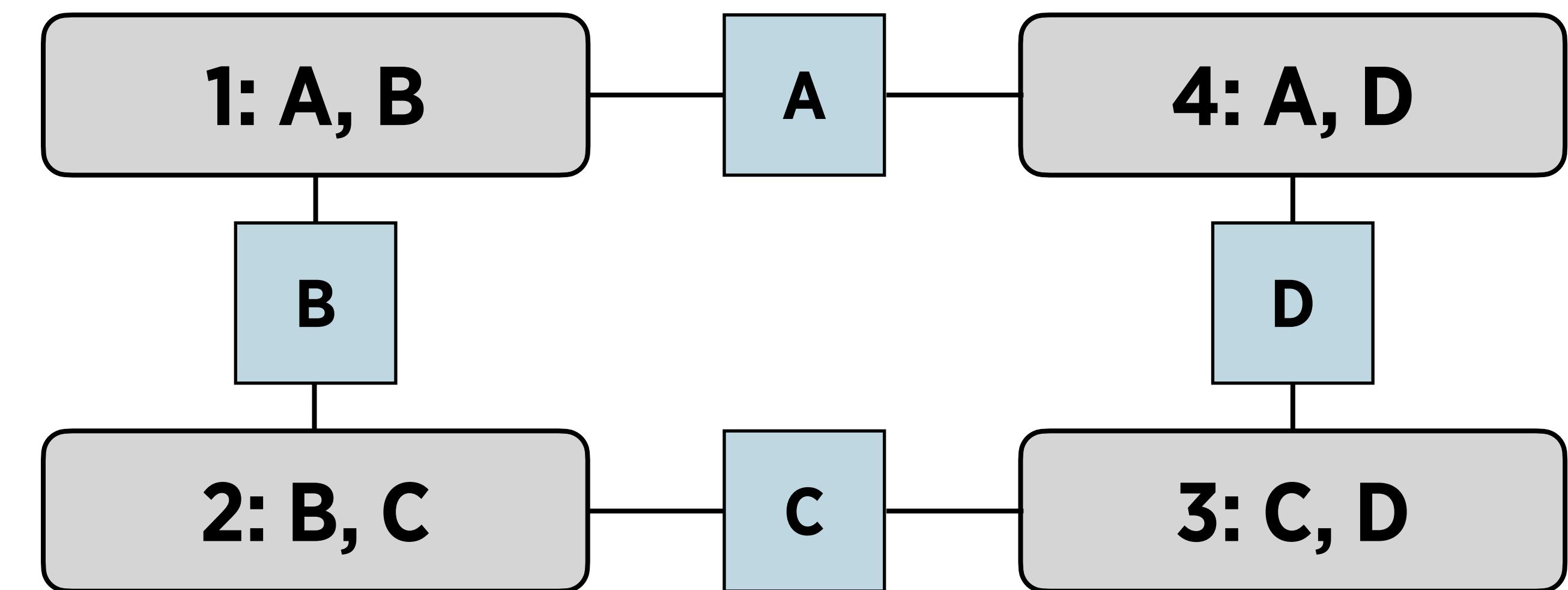
# Properties of BP Algorithm

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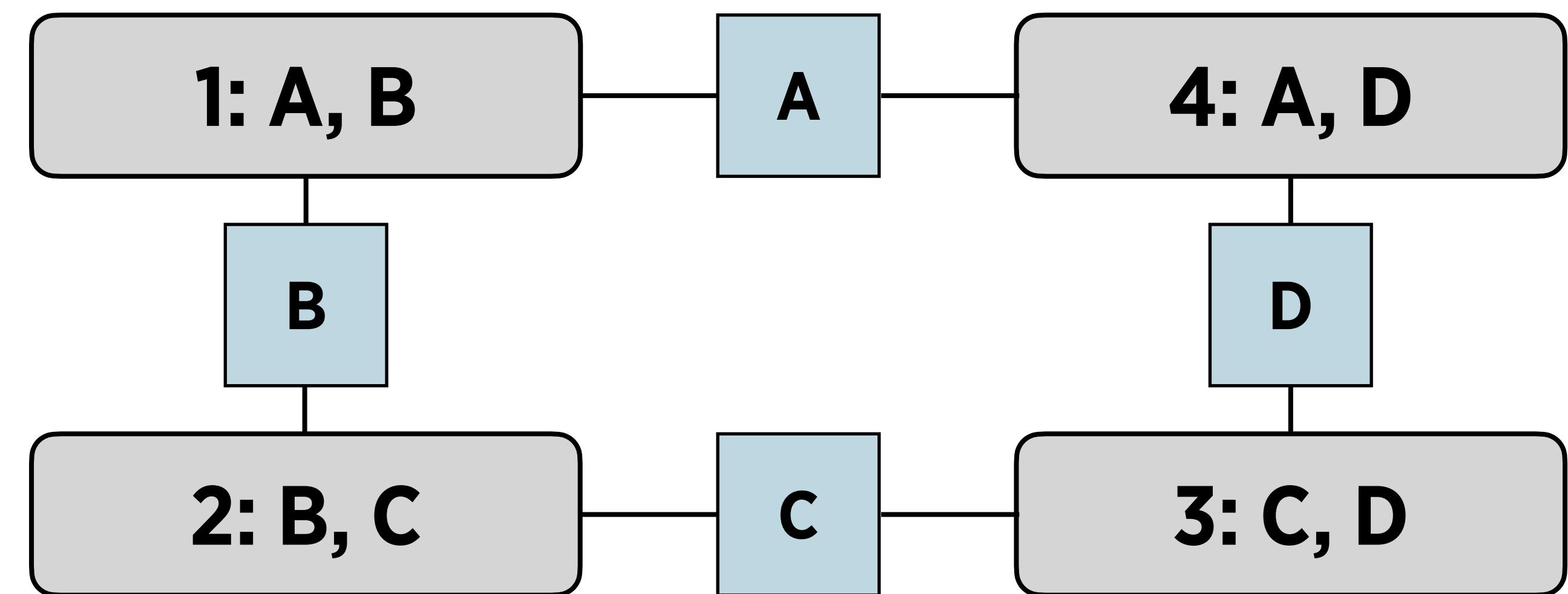
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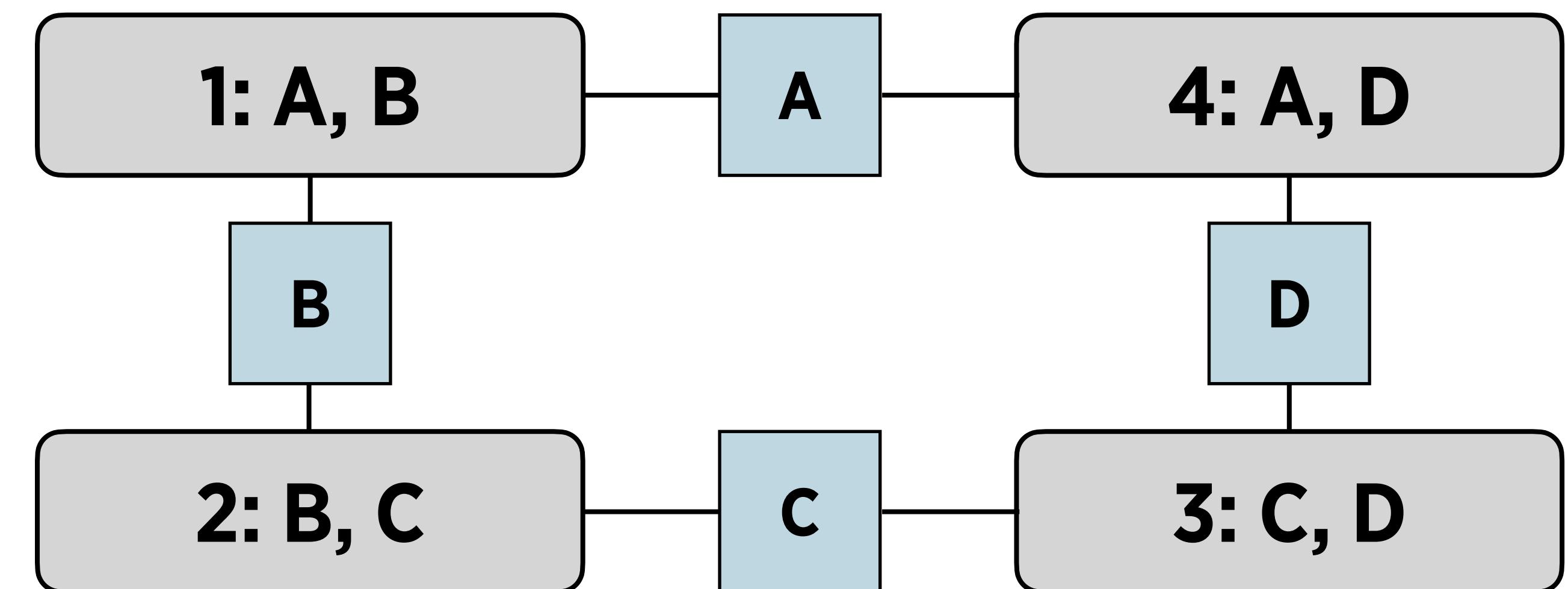


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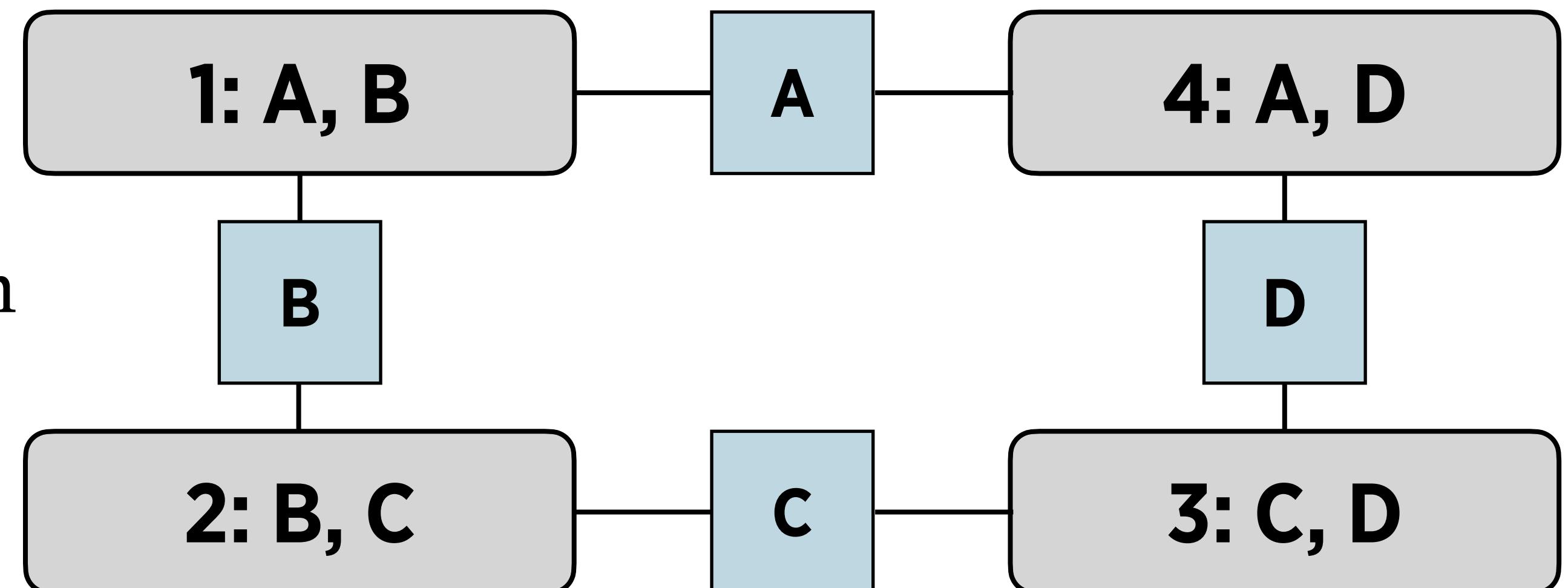
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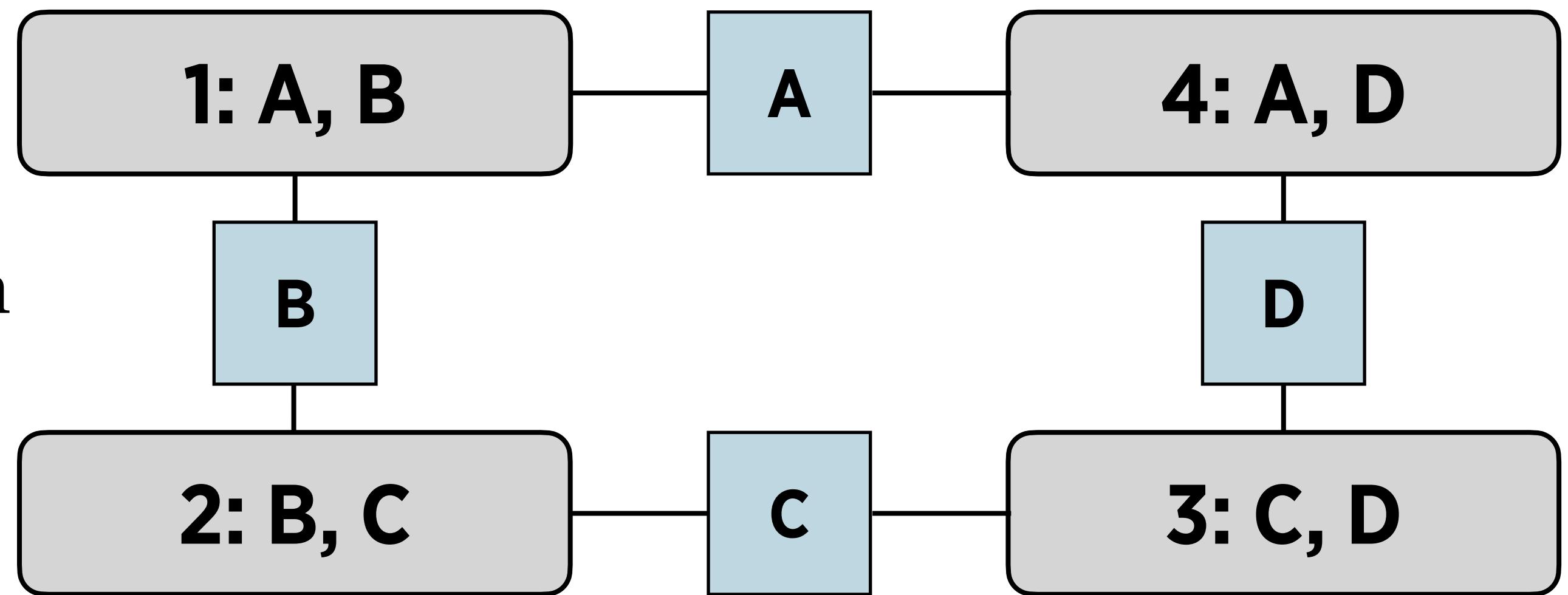
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$$\mu_{i,j}(\mathbf{S}_{i,j}) = \delta_{j \rightarrow i} \delta_{i \rightarrow j} = \sum_{\mathbf{C}_j - \mathbf{S}_{i,j}} \beta_j(\mathbf{C}_j)$$

# Convergence $\Rightarrow$ Calibration

$$\beta_i(\mathbf{C}_i) = \psi_i \times \prod_{k \in \mathcal{N}_i} \delta_{k \rightarrow i}$$

- Convergence:  $\delta_{i \rightarrow j}(\mathbf{S}_{i,j}) = \delta'_{i \rightarrow j}(\mathbf{S}_{i,j})$

$$- \delta'_{i \rightarrow j}(\mathbf{S}_{i,j}) = \sum_{\mathbf{C}_i - \mathbf{S}_{i,j}} \left( \psi_i \prod_{k \in (\mathcal{N}_i - \{j\})} \delta_{k \rightarrow i} \right) = \sum_{\mathbf{C}_i - \mathbf{S}_{i,j}} \frac{\beta_i(\mathbf{C}_i)}{\delta_{j \rightarrow i}(\mathbf{S}_{i,j})}$$

$$= \delta_{j \rightarrow i}(\mathbf{S}_{i,j}) \delta_{i \rightarrow j}(\mathbf{S}_{i,j}) = \sum_{\mathbf{C}_i - \mathbf{S}_{i,j}} \beta_i(\mathbf{C}_i)$$

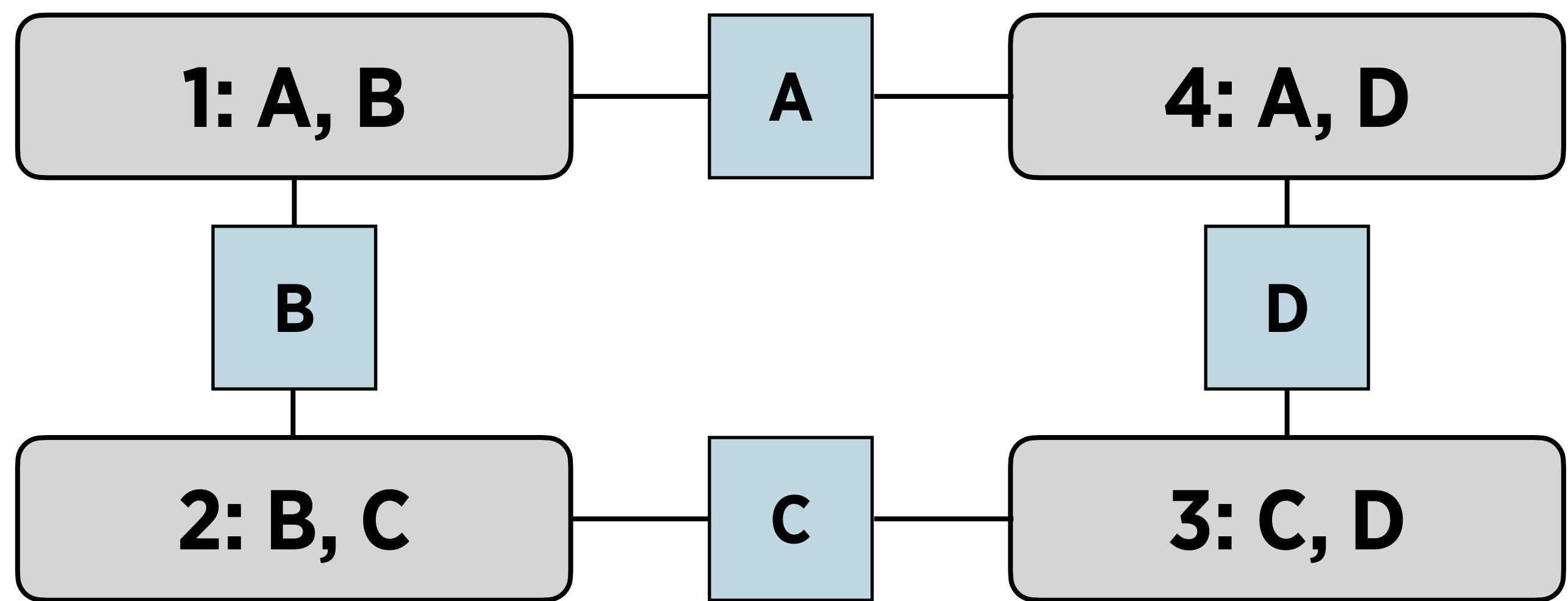
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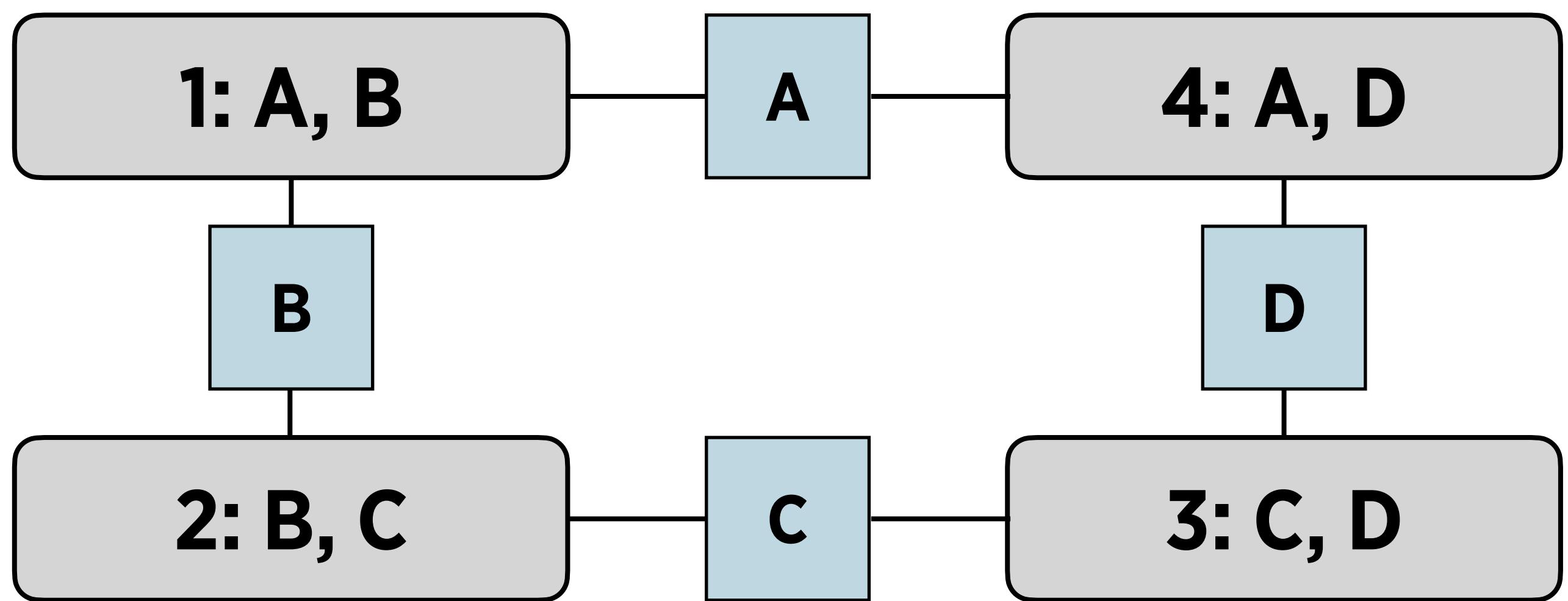
sepset belief

# Reparameterisation



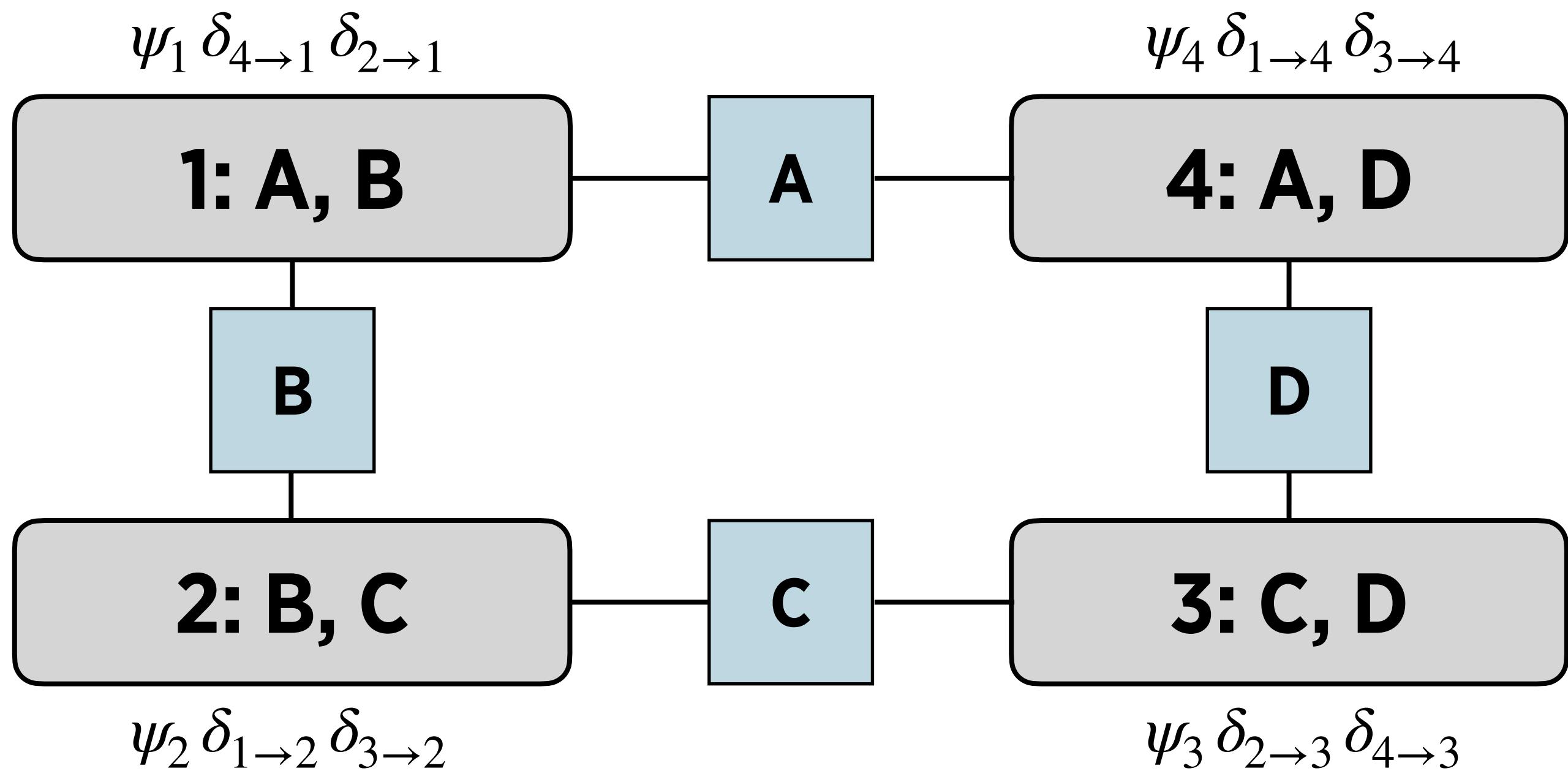
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$$\beta_i(C_i) = \psi_i \prod_{k \in \mathcal{N}_i} \delta_{k \rightarrow i}$$



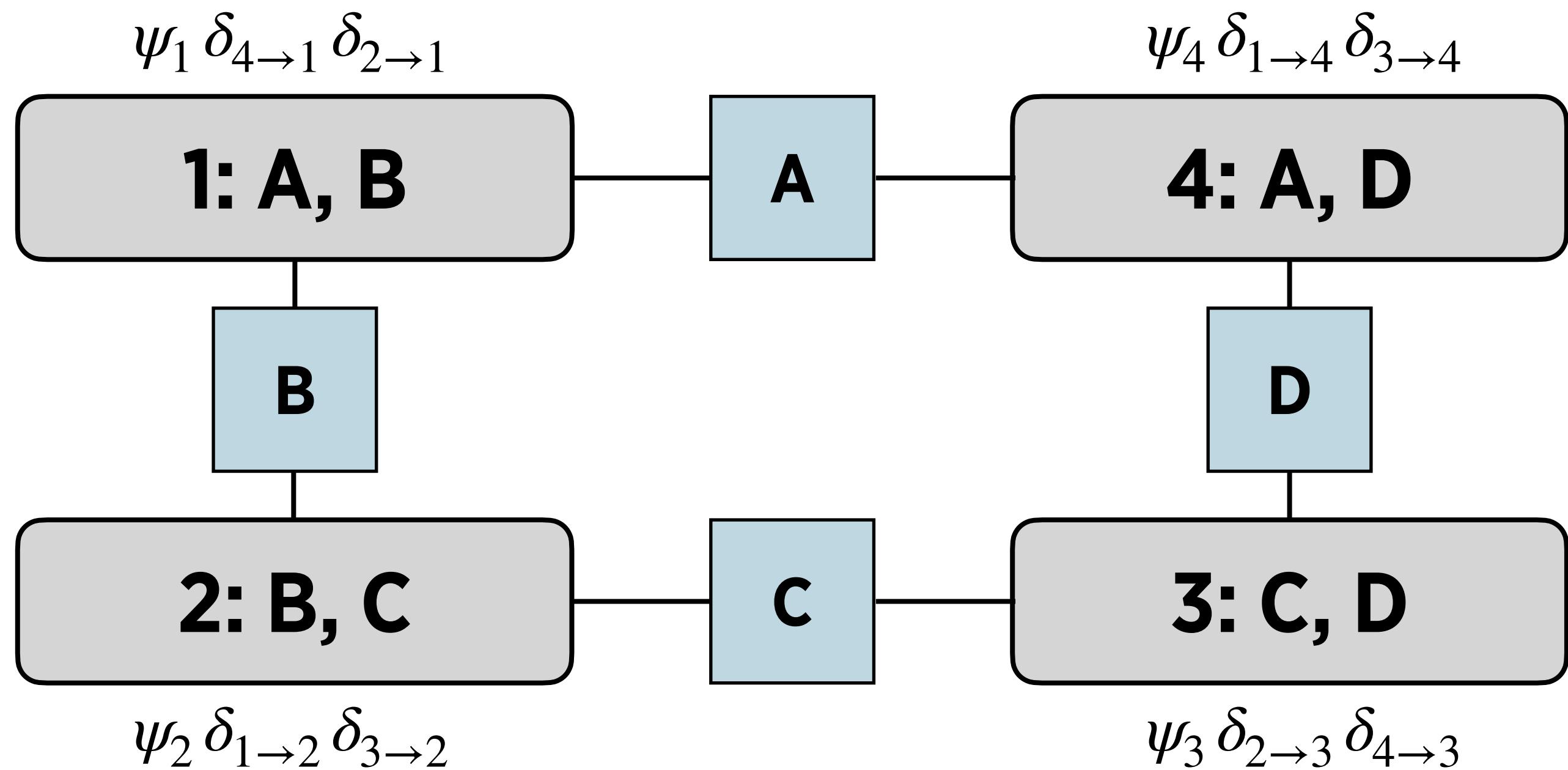
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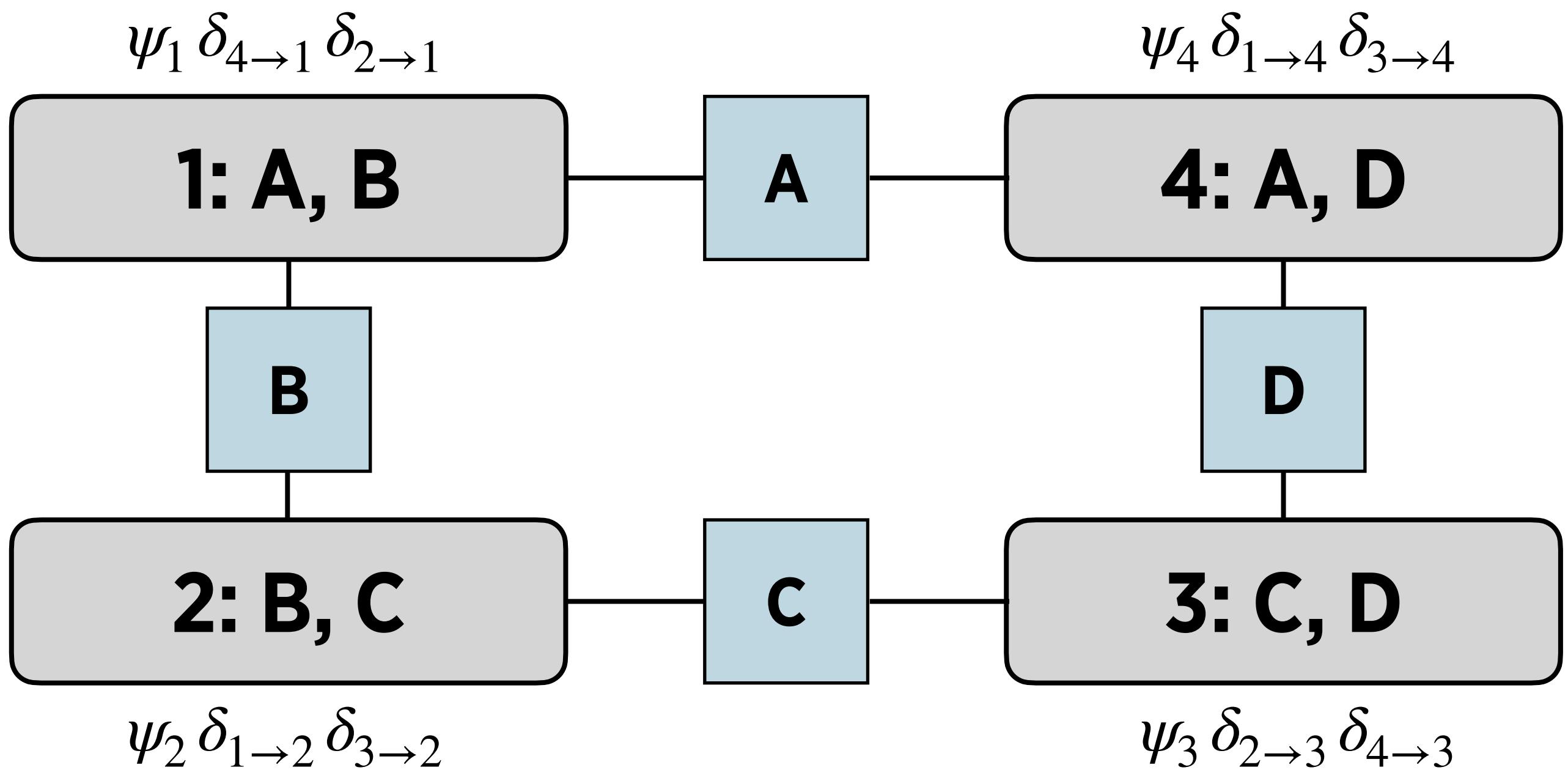
$$\beta_i(C_i) = \psi_i \prod_{k \in \mathcal{N}_i} \delta_{k \rightarrow i} \quad \mu_{i,j}(S_{i,j}) = \delta_{j \rightarrow i} \delta_{i \rightarrow j}$$



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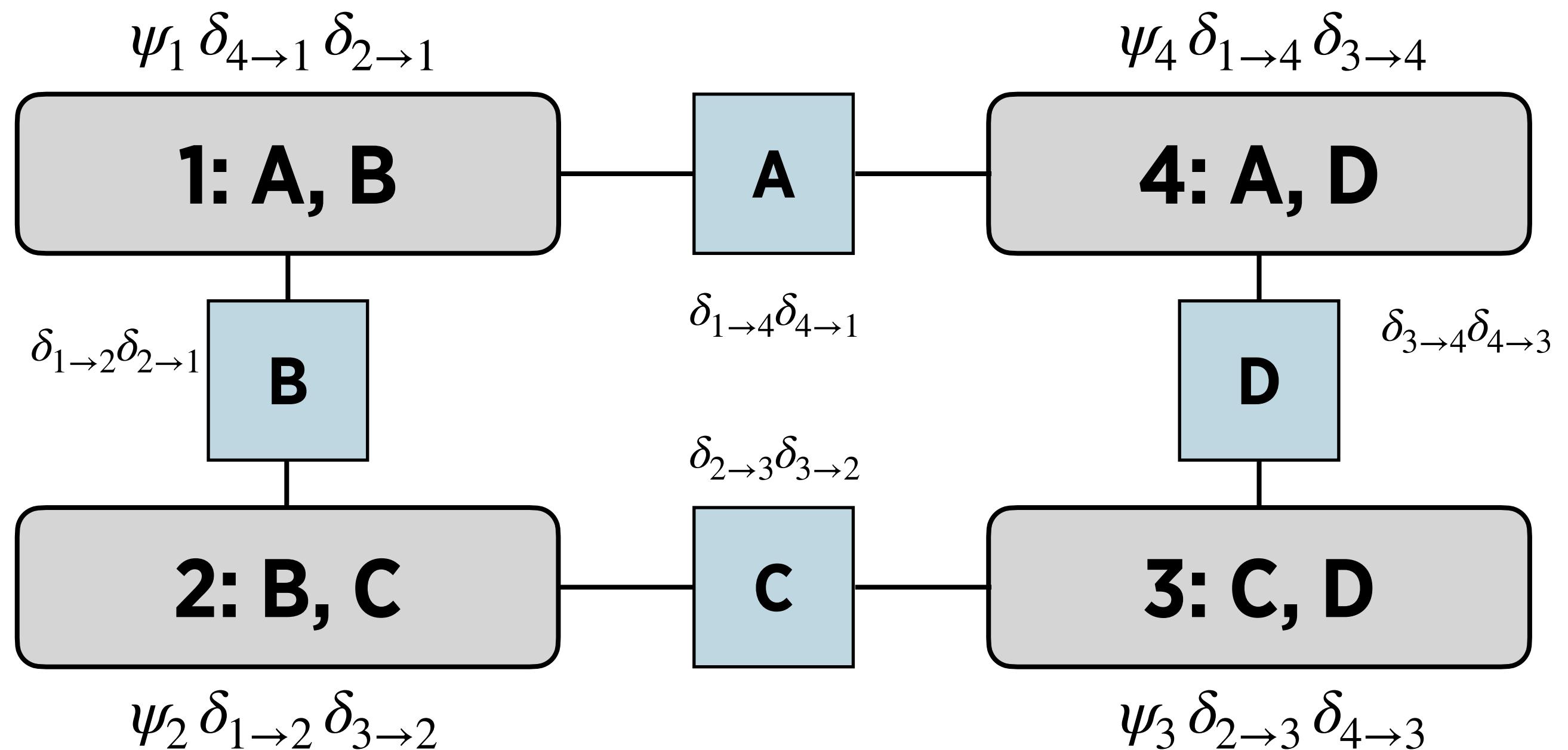
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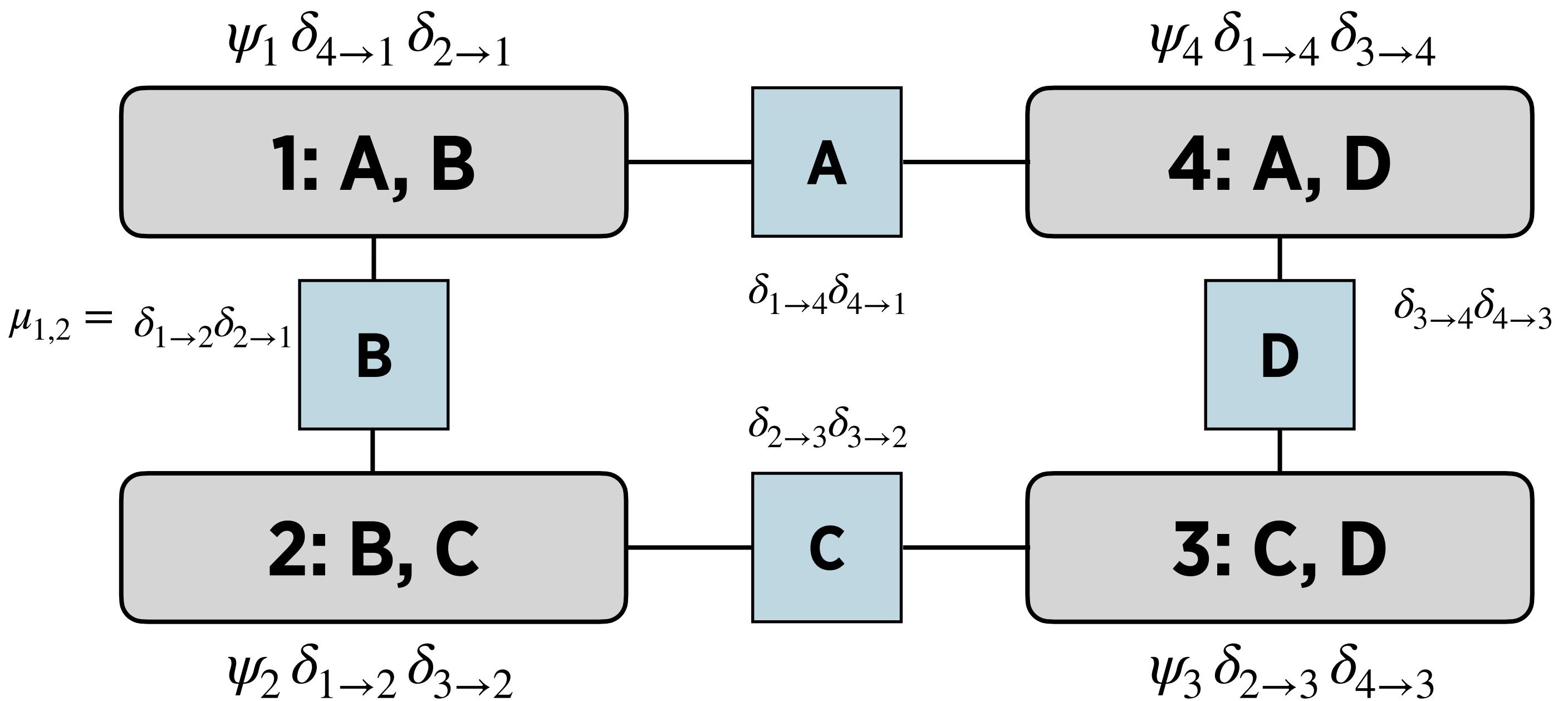
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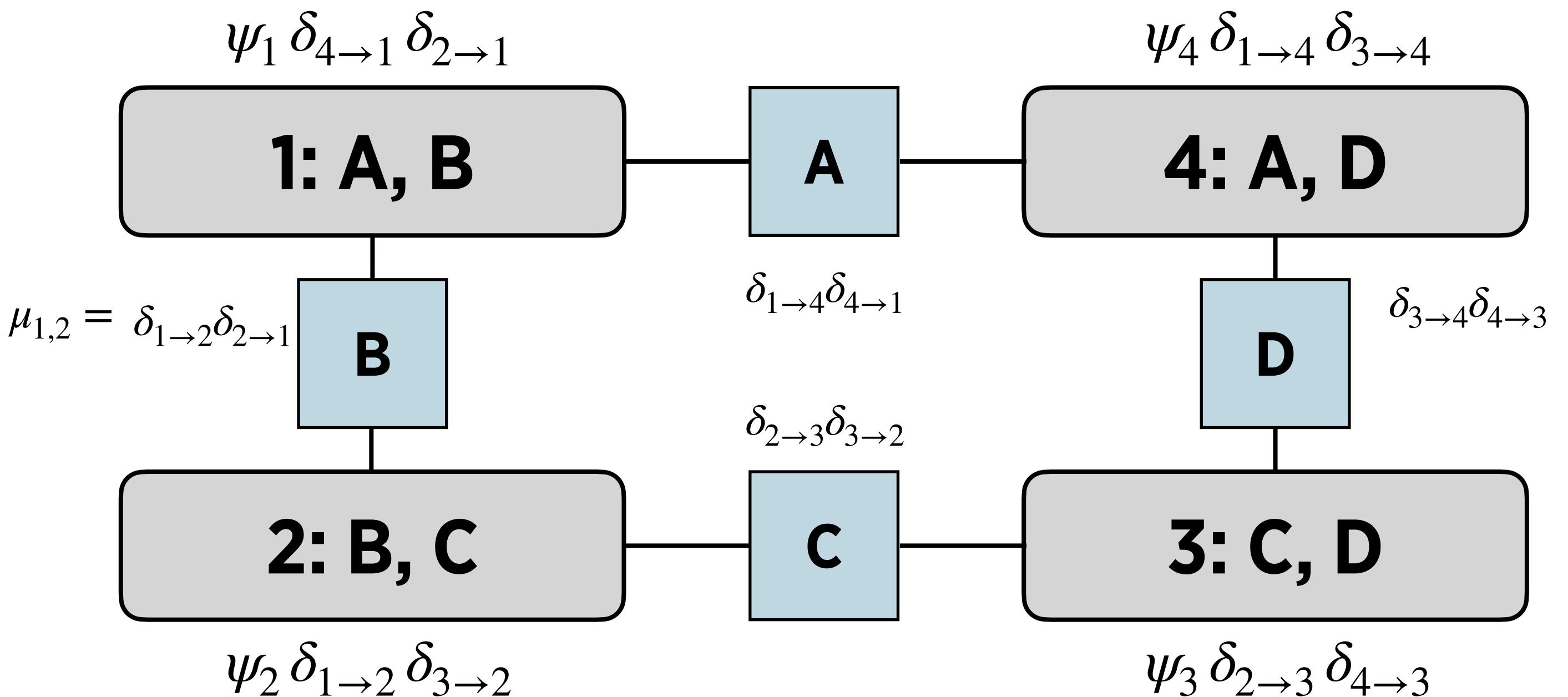


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sepset belief

$$\frac{\prod_i \beta_i}{\prod_{i,j} \mu_{i,j}}$$



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$$= \prod_i \psi_i = \tilde{P}_{\Phi}(X_1, \dots, X_n)$$

# Summary Properties of Belief Propagation

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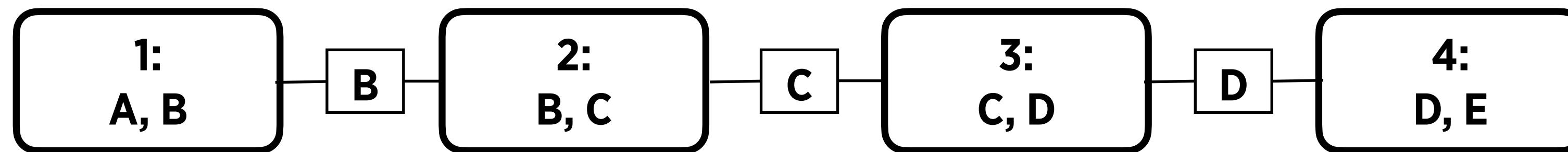
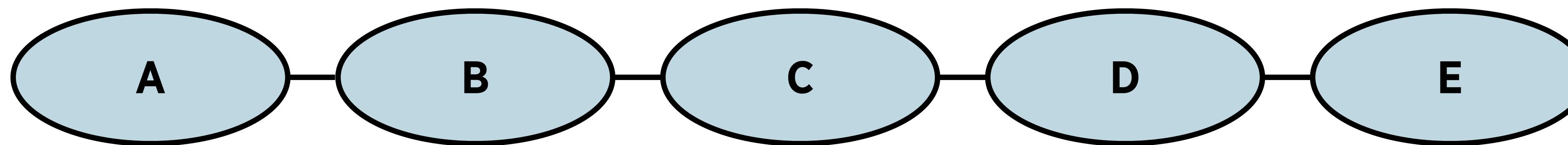
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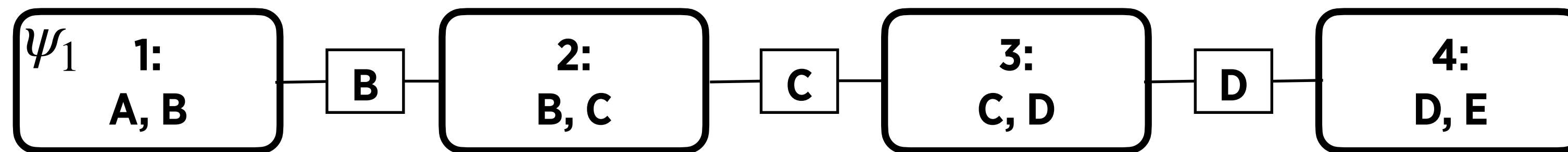
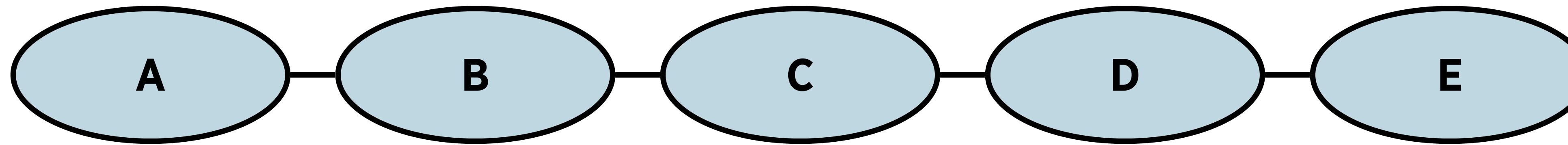
- At convergence of BP, cluster graph beliefs are calibrated:
- Beliefs at adjacent clusters agree on sepsets
- Cluster graph beliefs are an alternative calibrated parameterisation of the original unnormalised density
- No information is lost by message passing

# Clique Tree Algorithm & Correctness

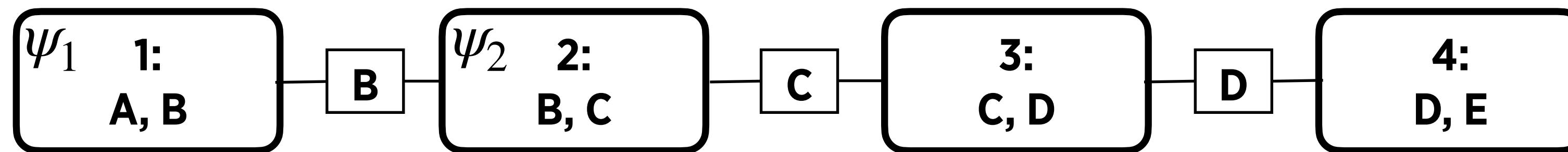
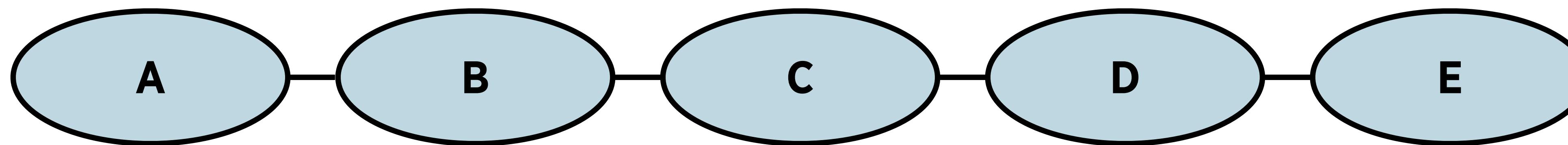
# Message Passing in Trees



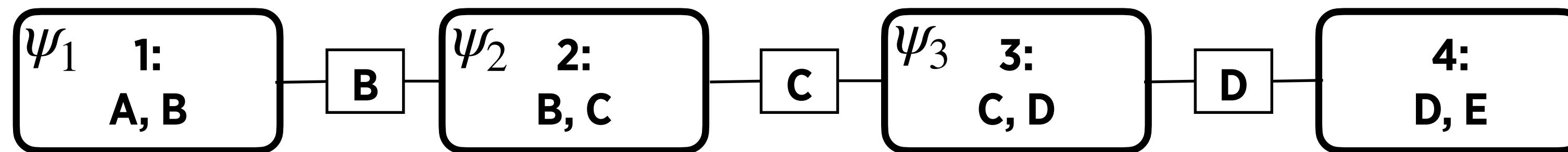
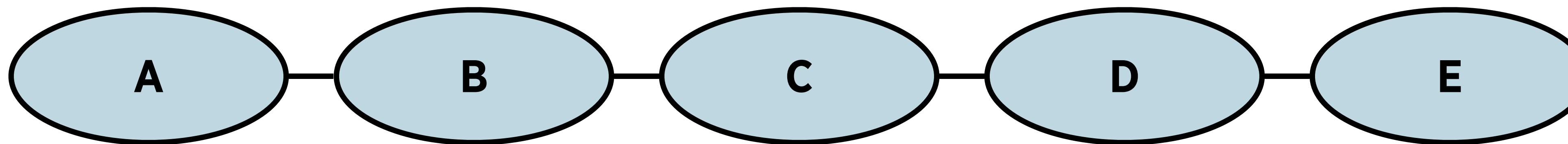
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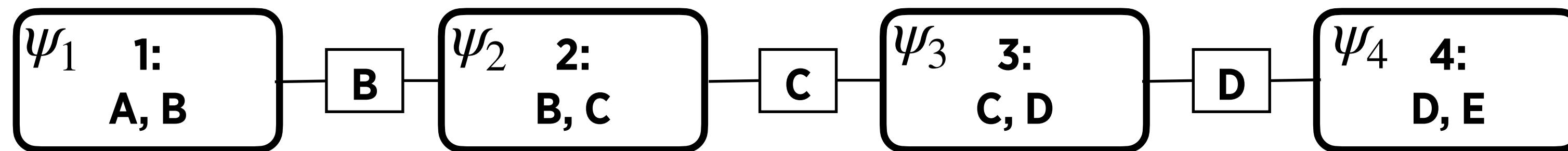
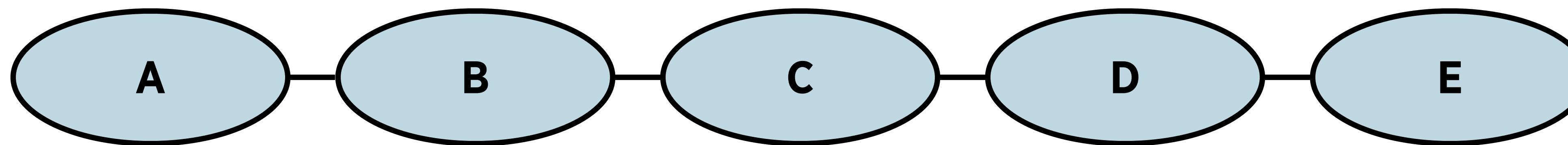
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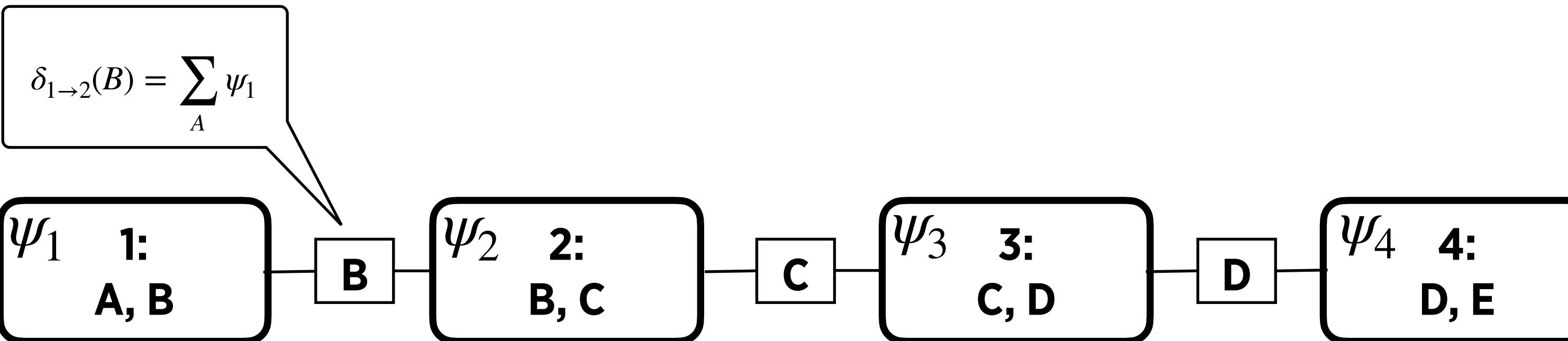
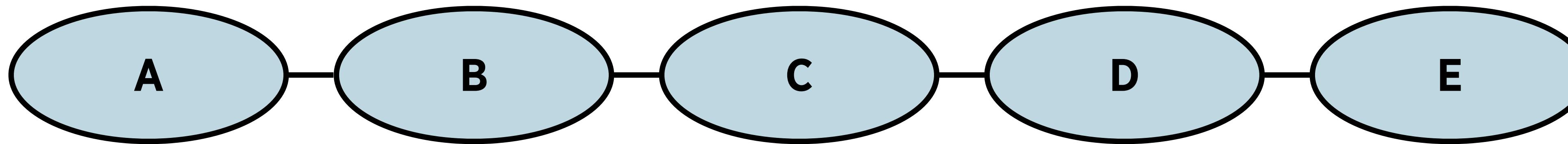
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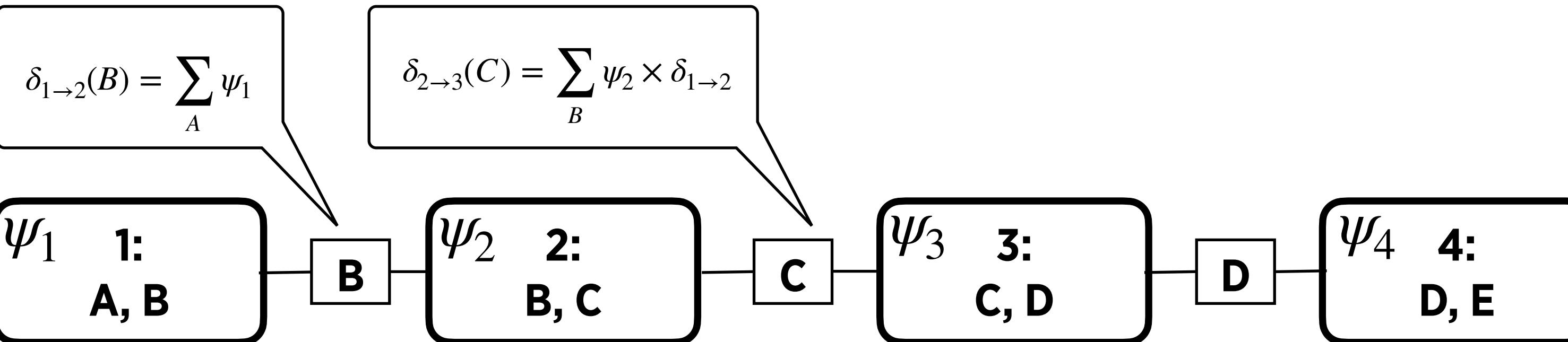
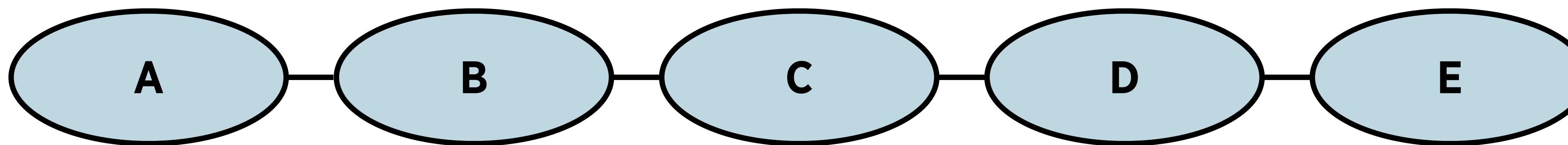
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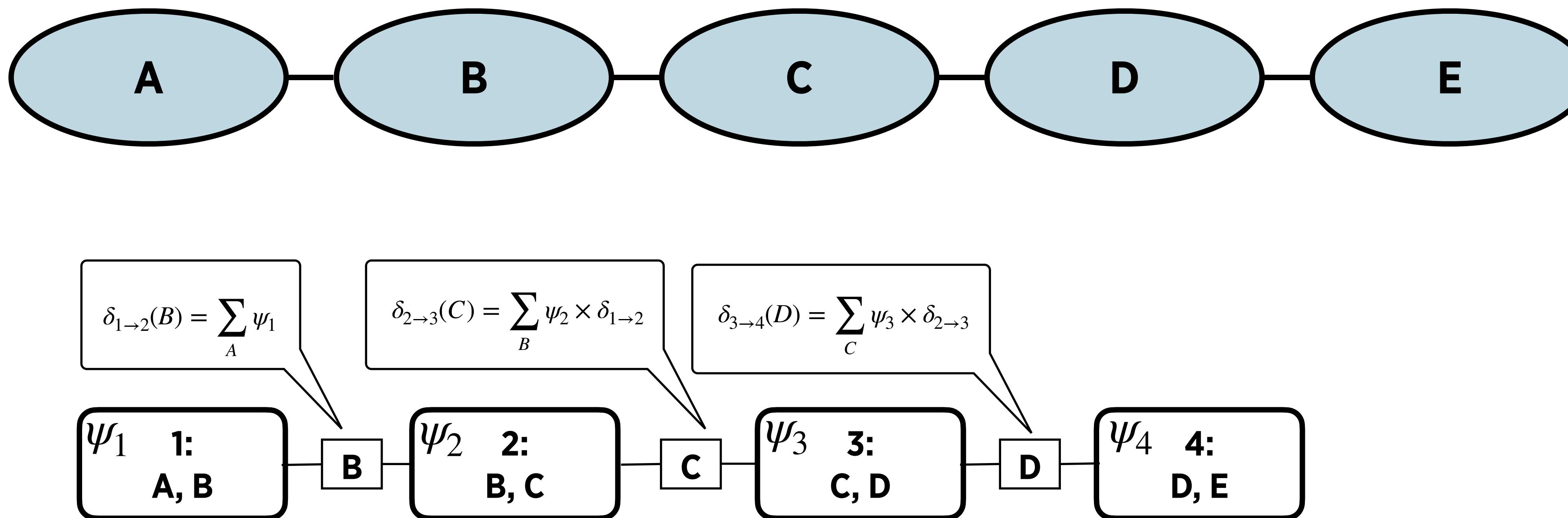
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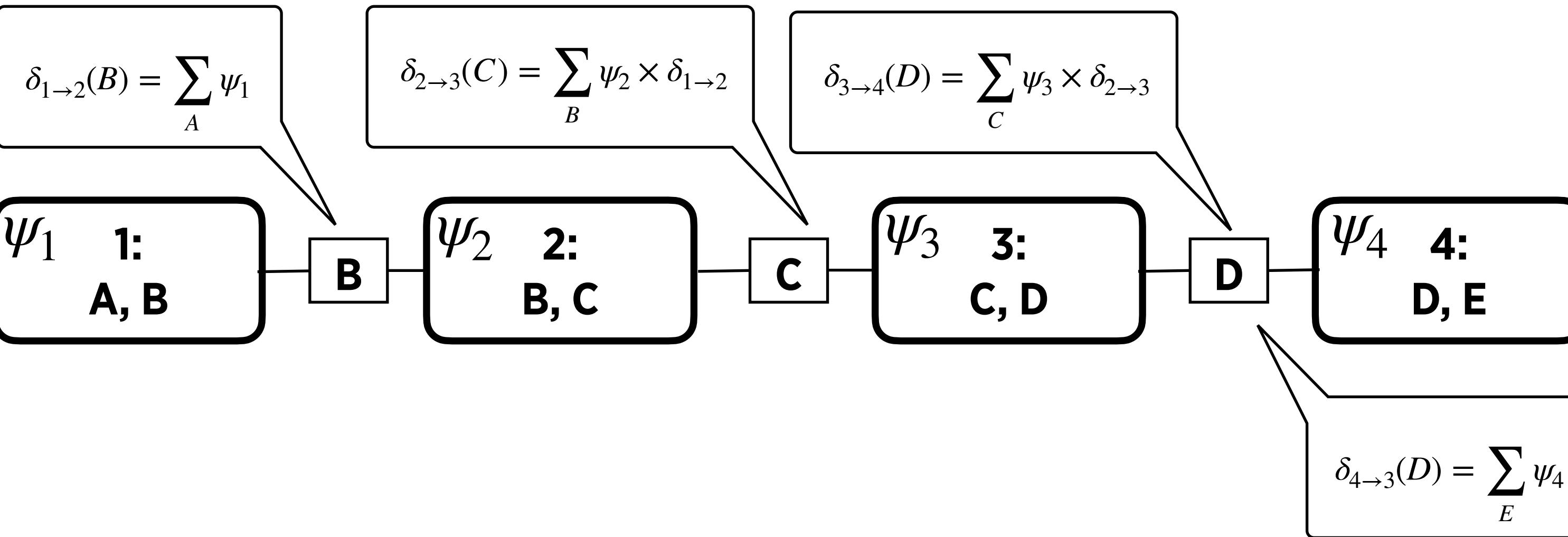
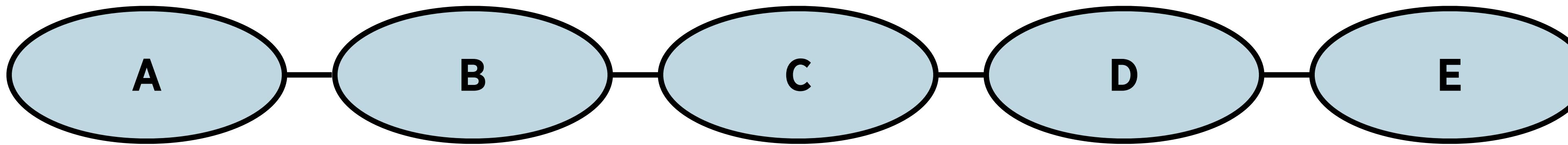
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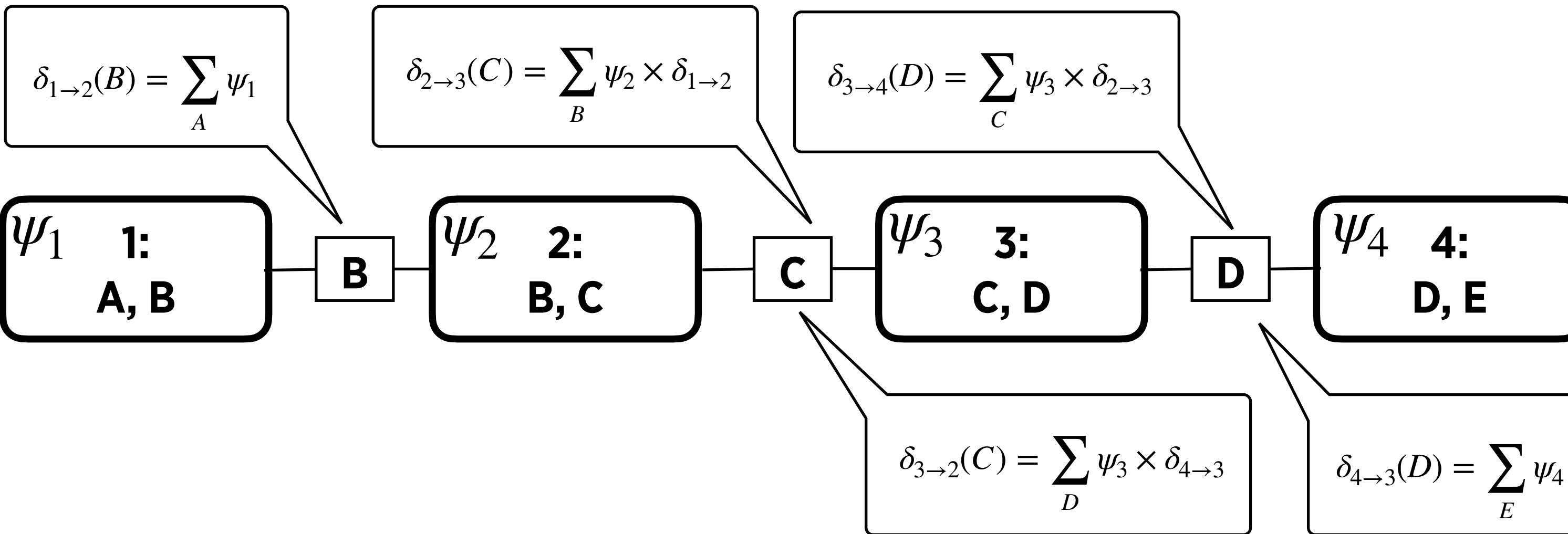
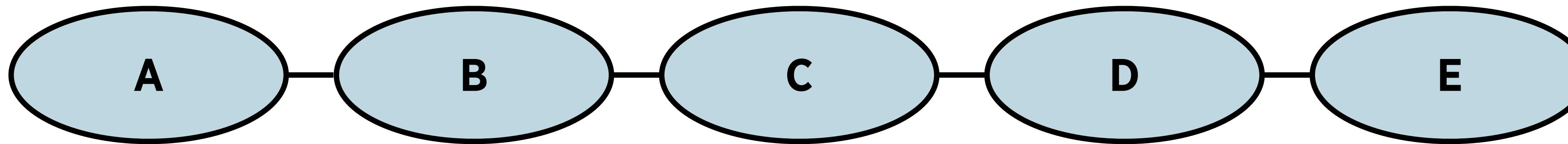
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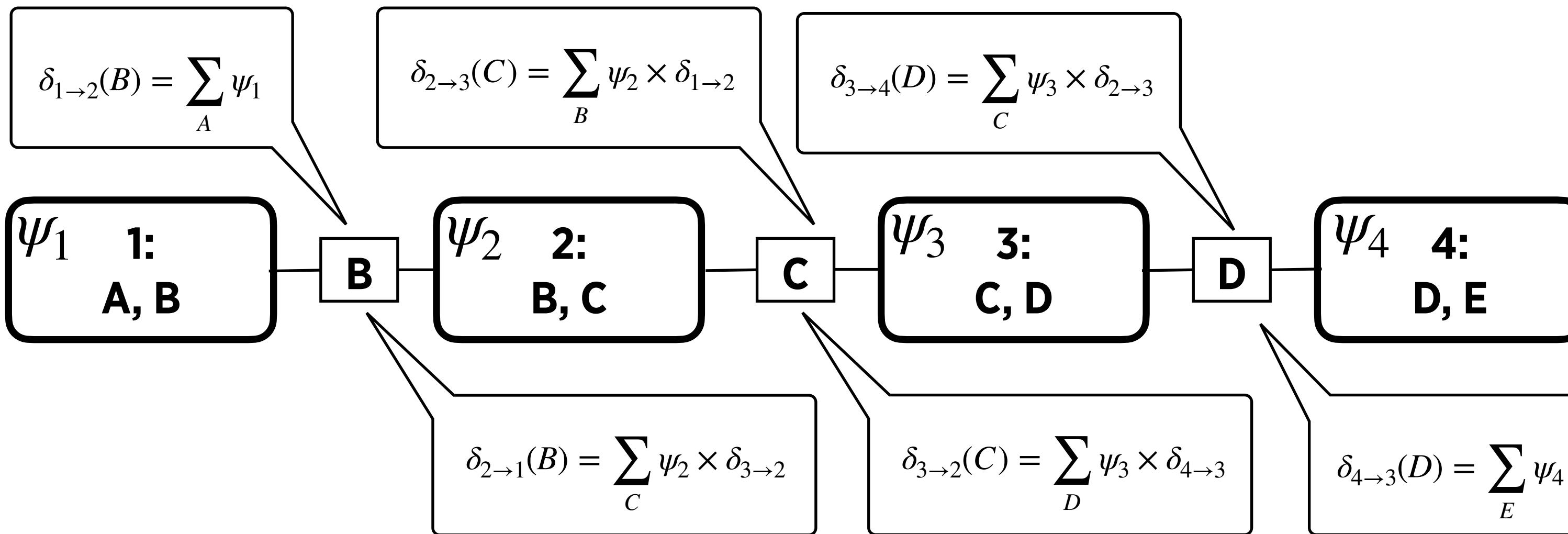
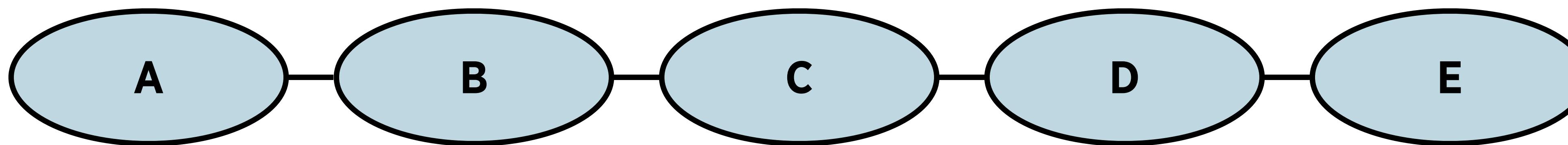
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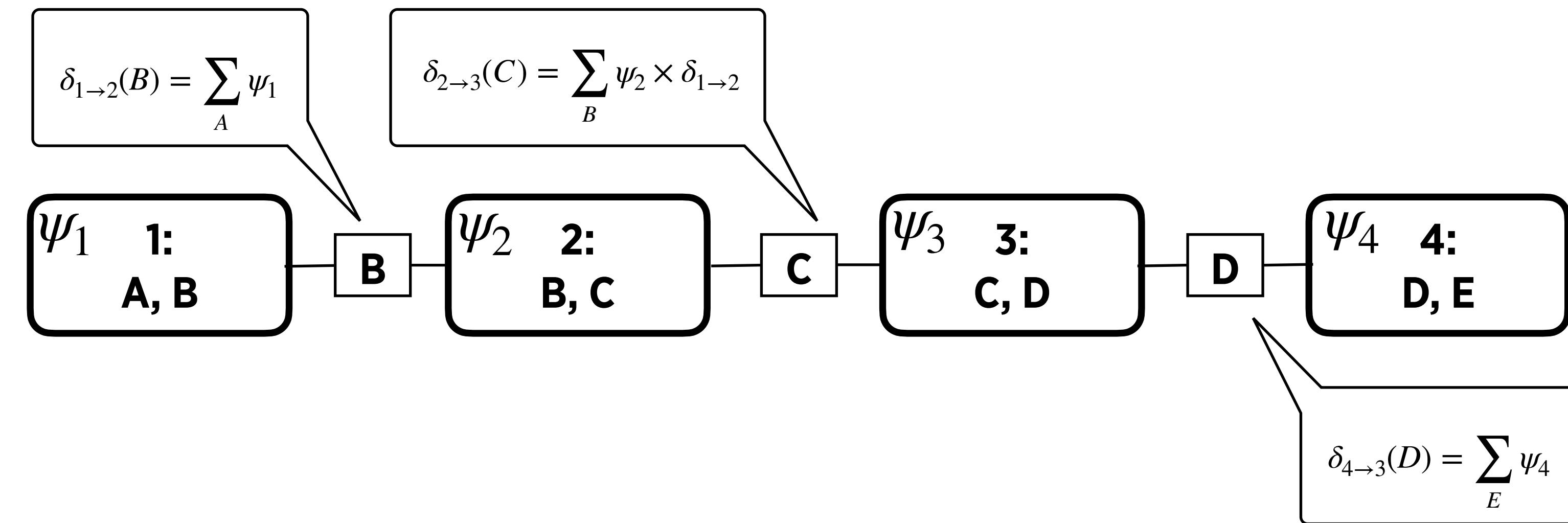
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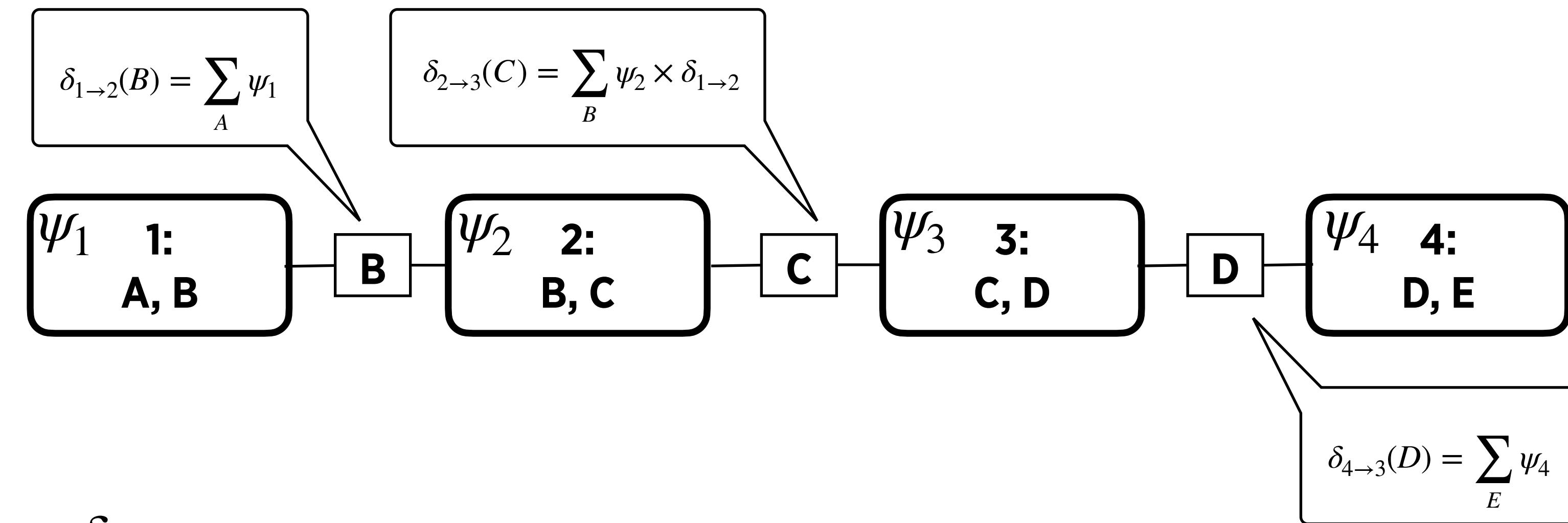
# Message Passing in Trees



# Correctness

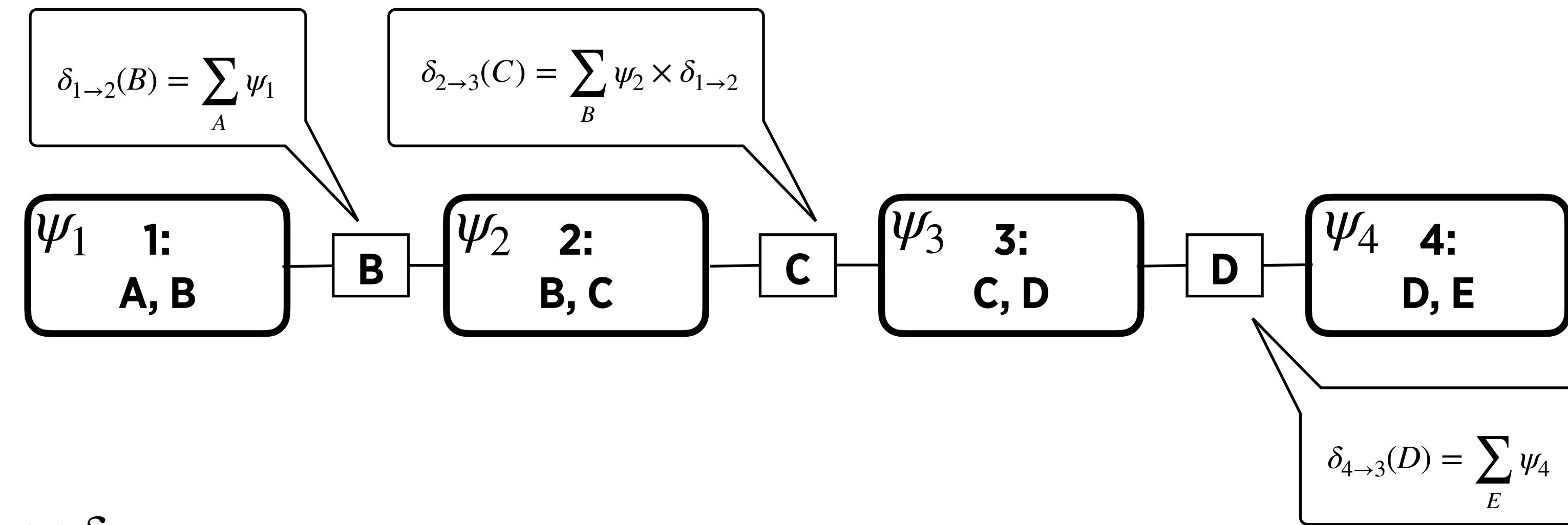


# Correctness



$$\beta_3(C, D) = \psi_3 \times \delta_{2 \rightarrow 3} \times \delta_{4 \rightarrow 3}$$

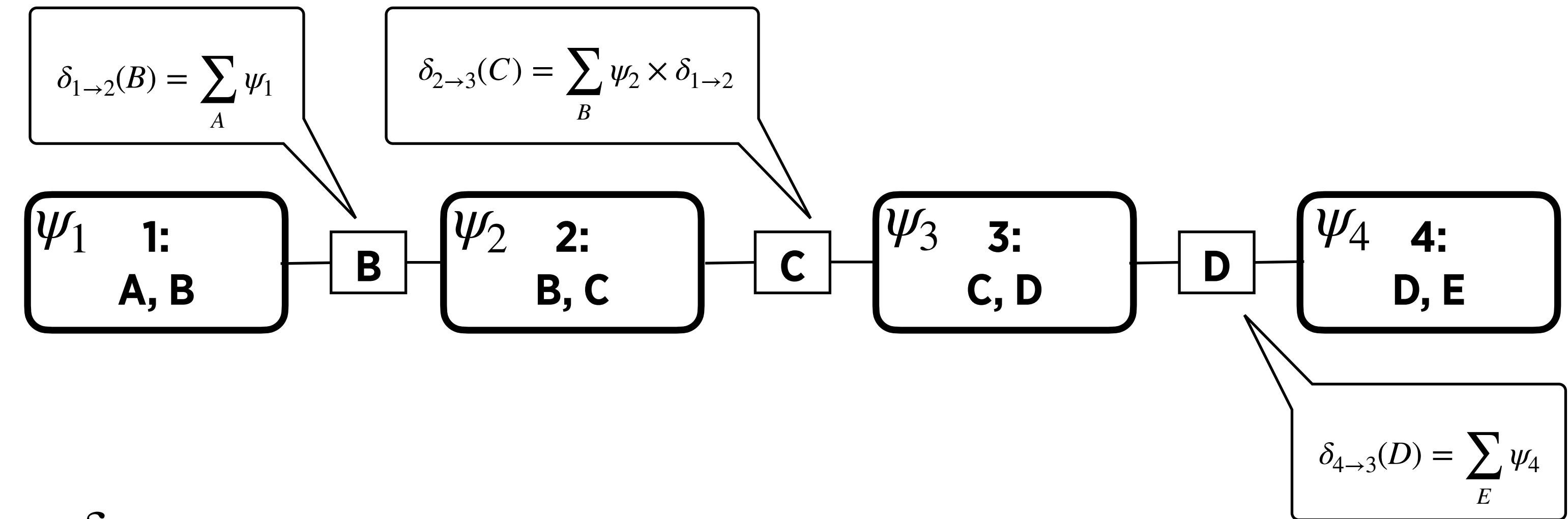
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# Clique Tree

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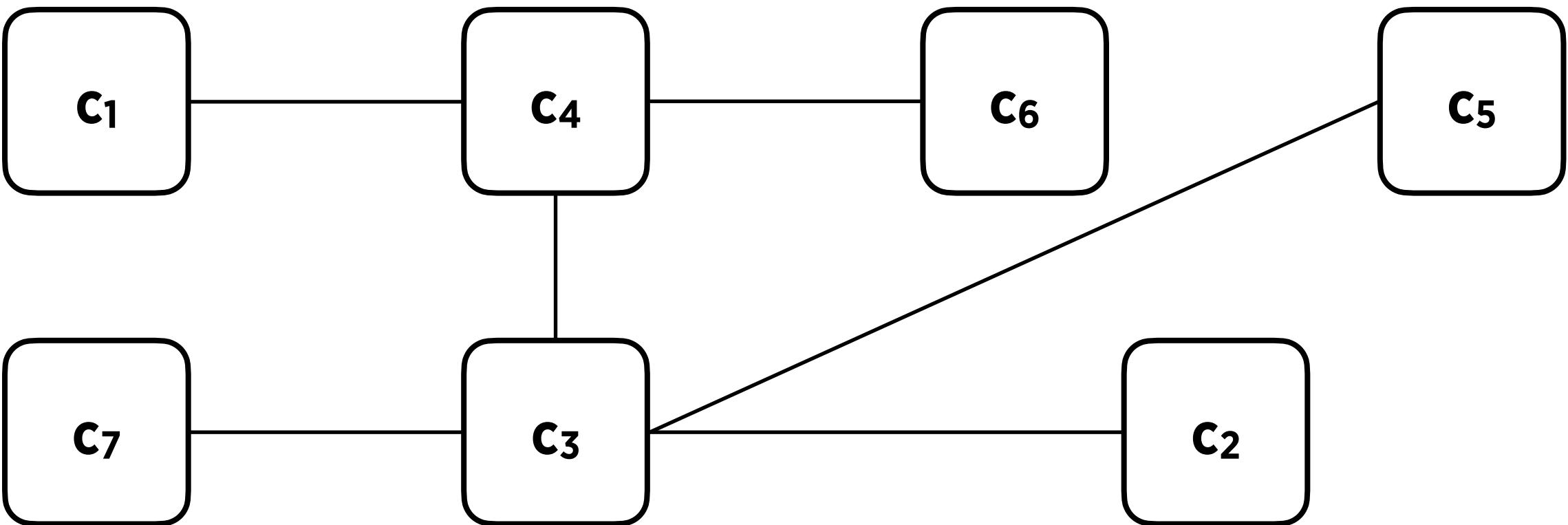
- Undirected tree such that
  - Nodes are clusters  $C_i \subseteq \{X_1, \dots, X_n\}$
  - Edge between  $C_i$  and  $C_j$  associated with sepset  $S_{i,j} = C_i \cap C_j$

# Family Preservation

- Given set of factors  $\Phi$ , we assign each  $\phi_k \in \Phi$  to a cluster  $C_{\alpha(k)}$  s.t.  $\text{scope}[\alpha_k] \subseteq C_{\alpha(k)}$
- For each factor  $\phi_k \in \Phi$ , there exists a cluster  $C_i$  s.t.  $\text{scope}[\phi_k] \subseteq C_i$

# Running Intersection Property

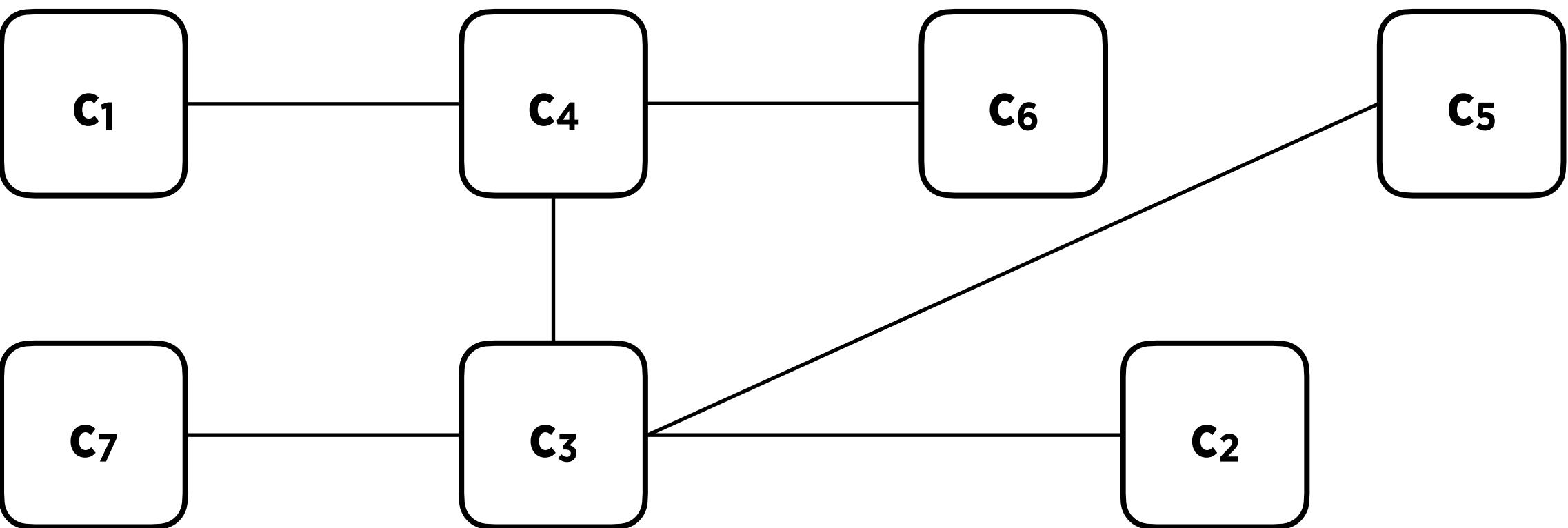
- For each pair of clusters  $C_i, C_j$  and variable  $X \in C_i \cap C_j$  there exists a unique path between  $C_i$  and  $C_j$  for which all clusters and sepsets contain  $X$



# Running Intersection Property

Cluster graph variant of the property

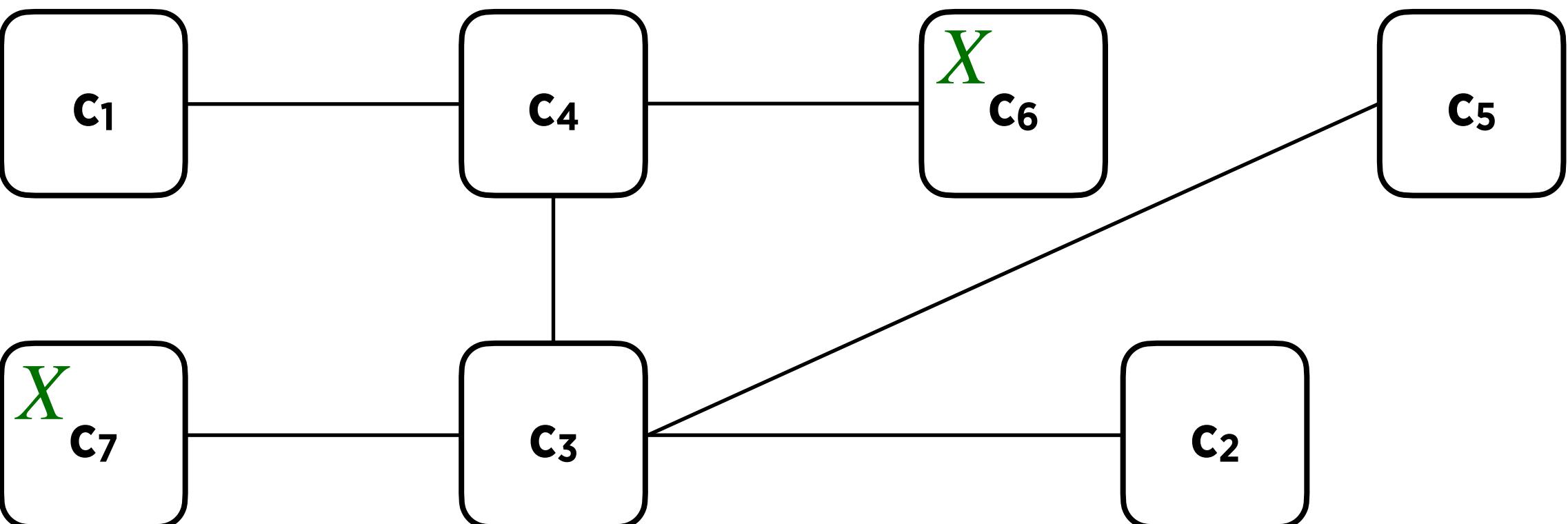
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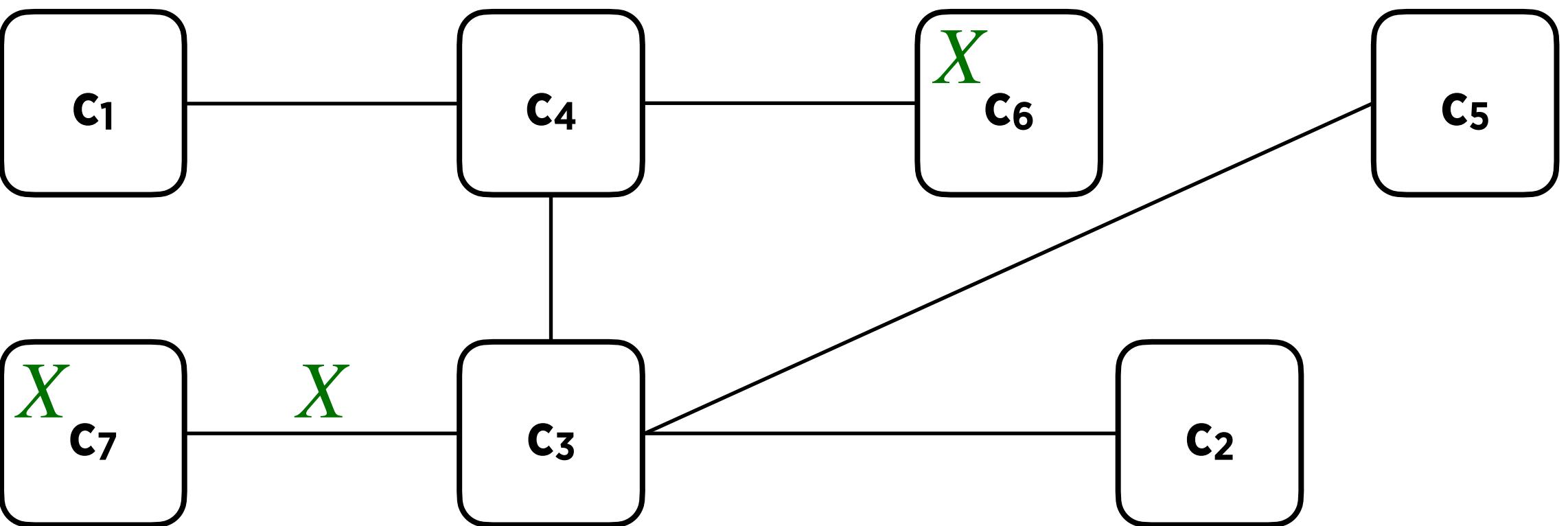
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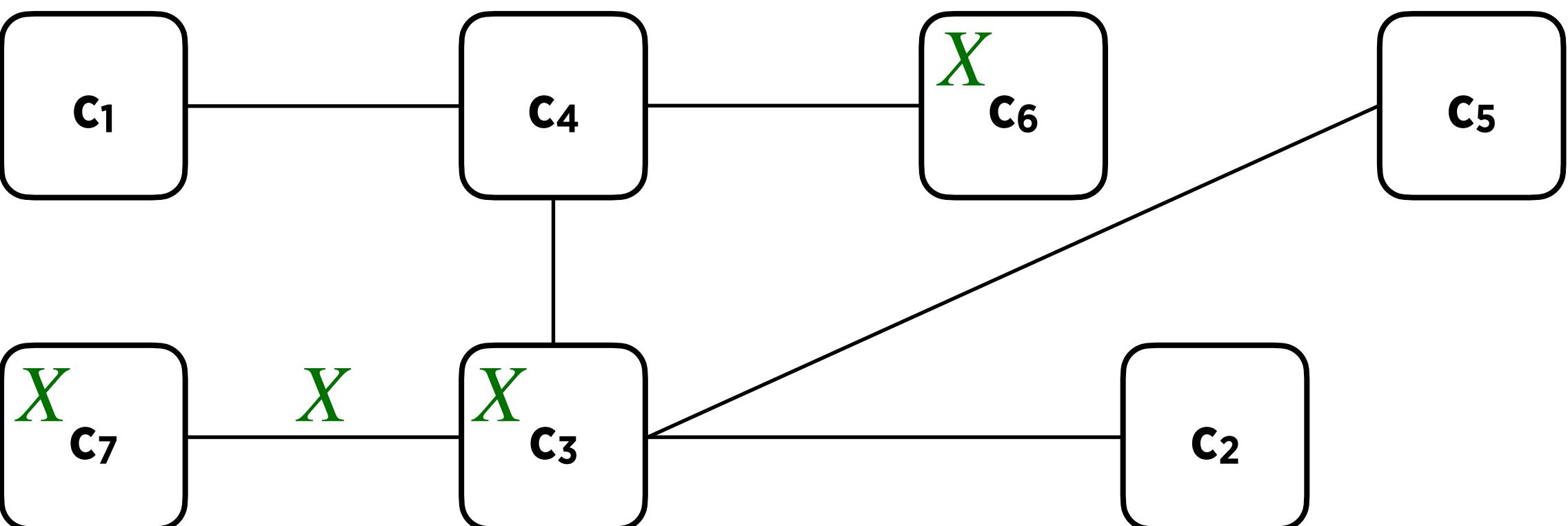
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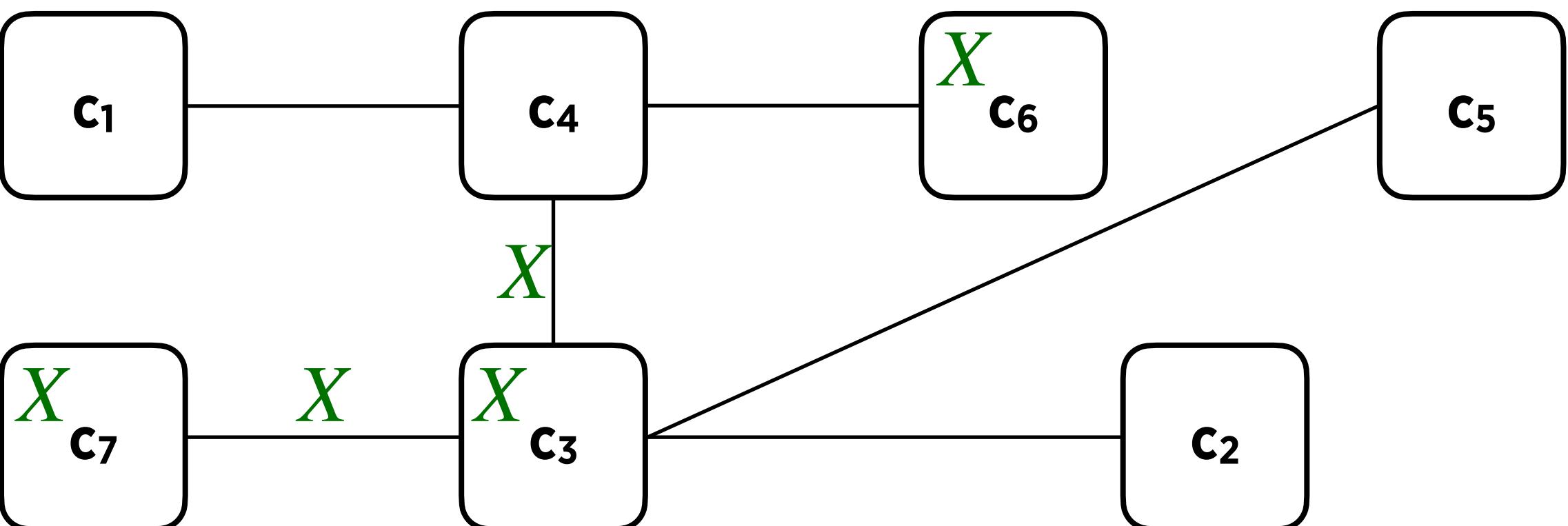
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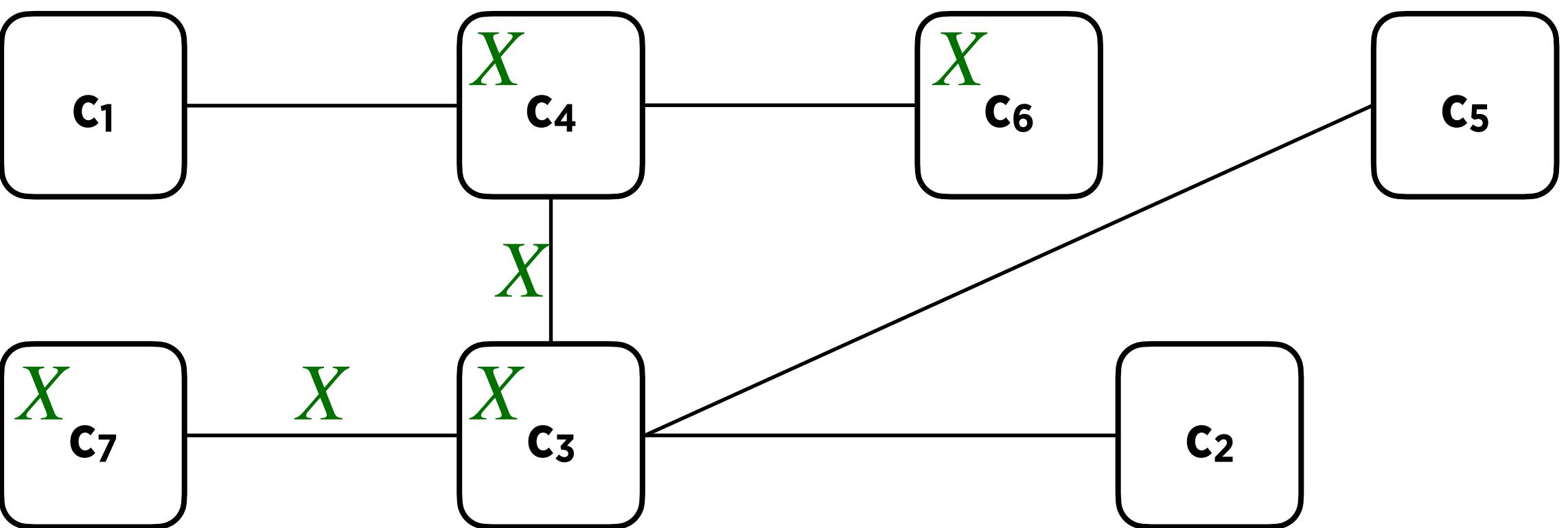
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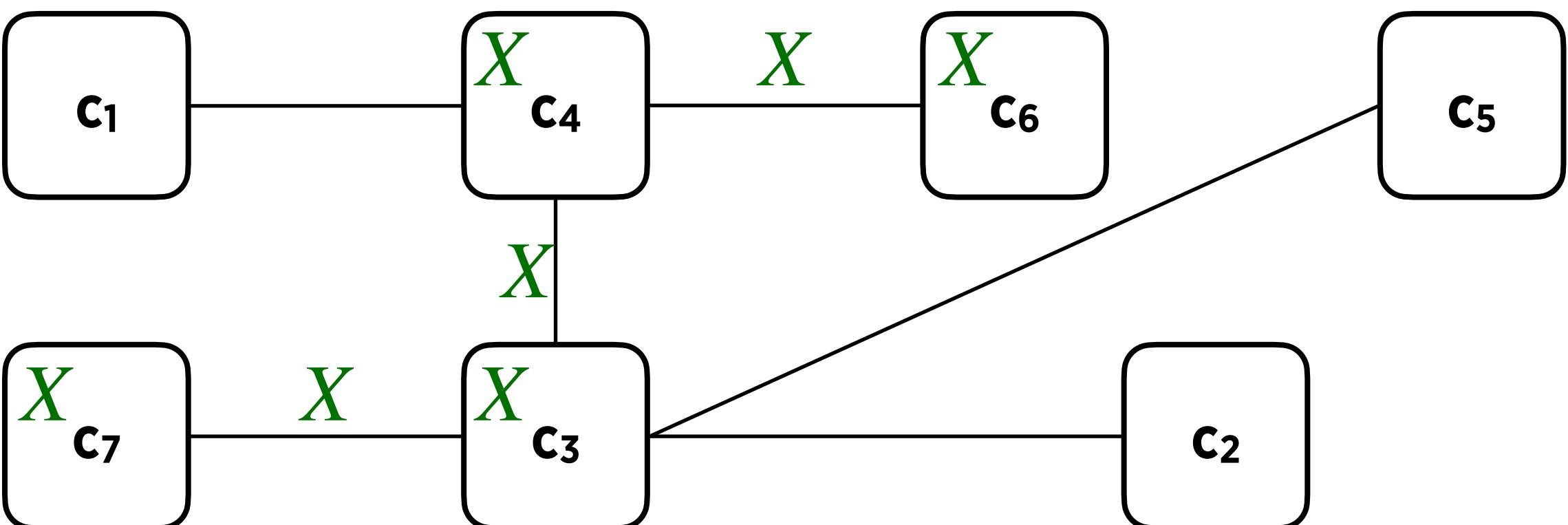
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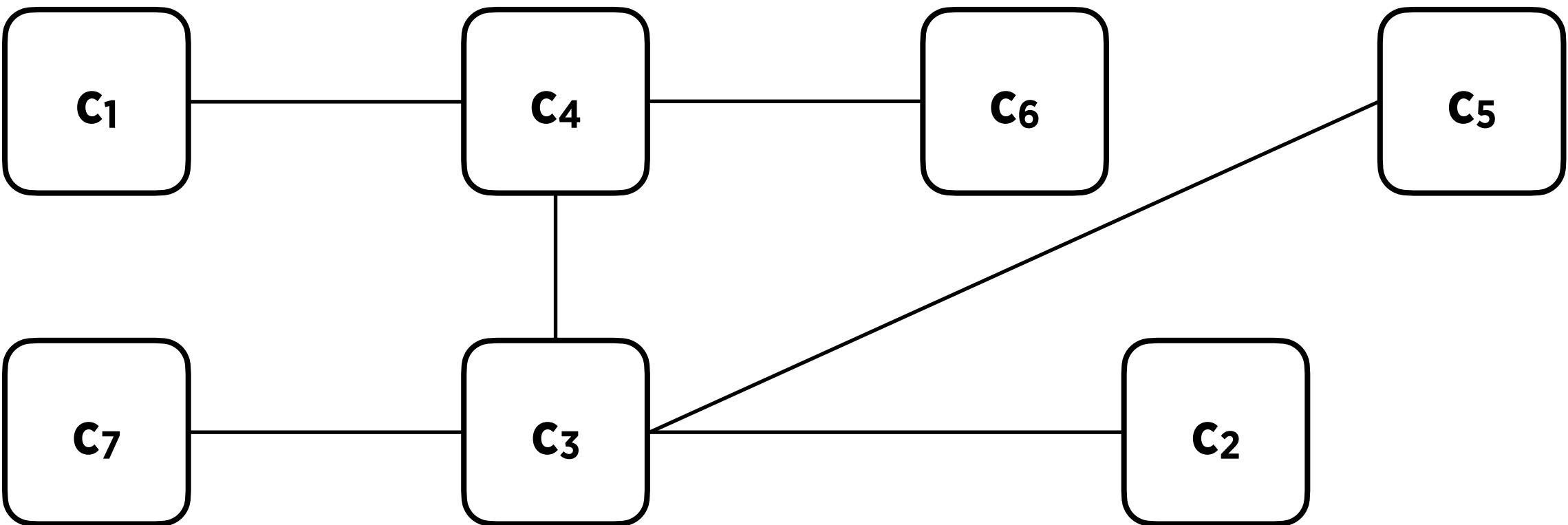
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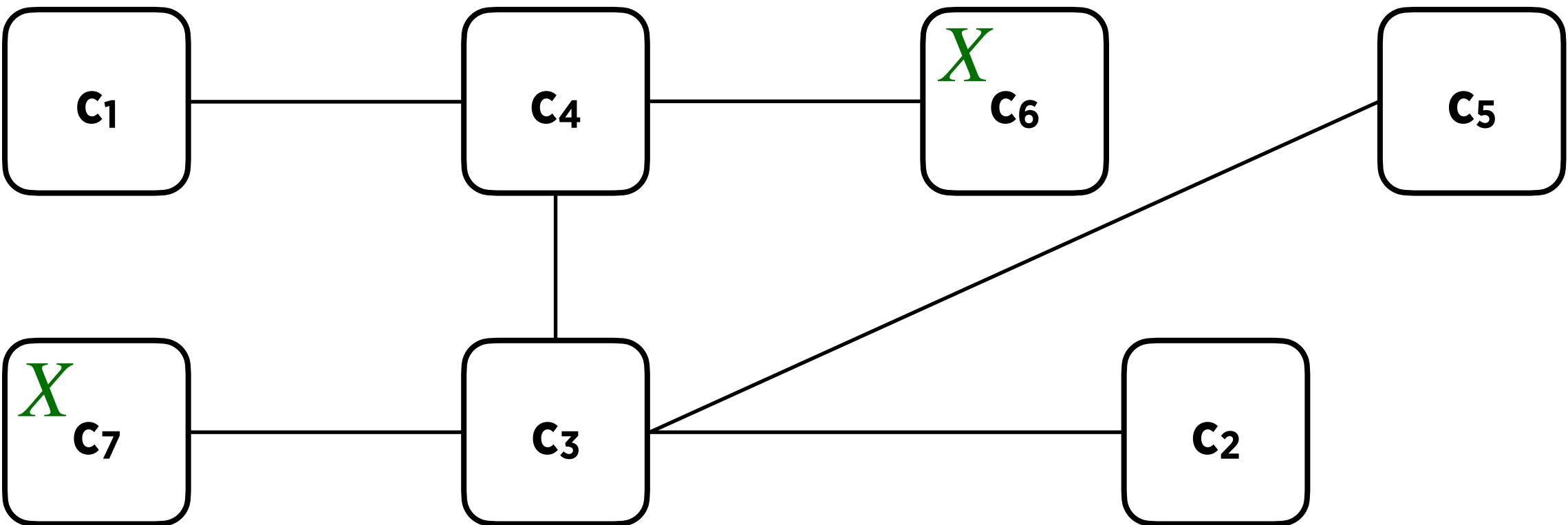
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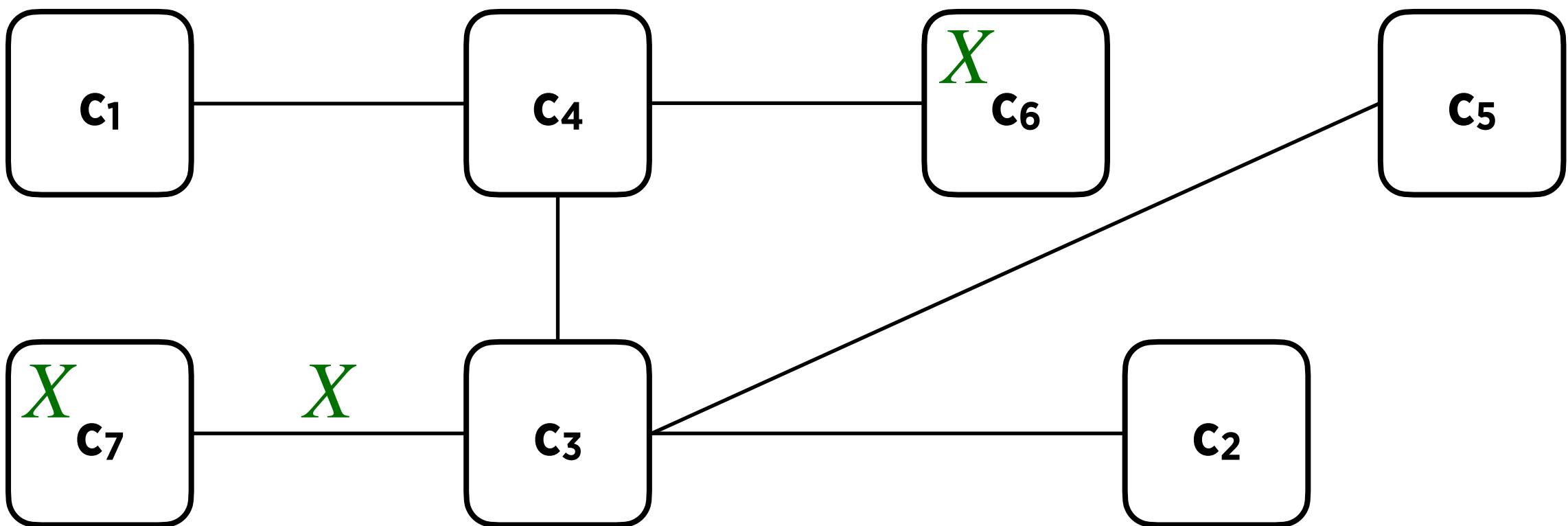
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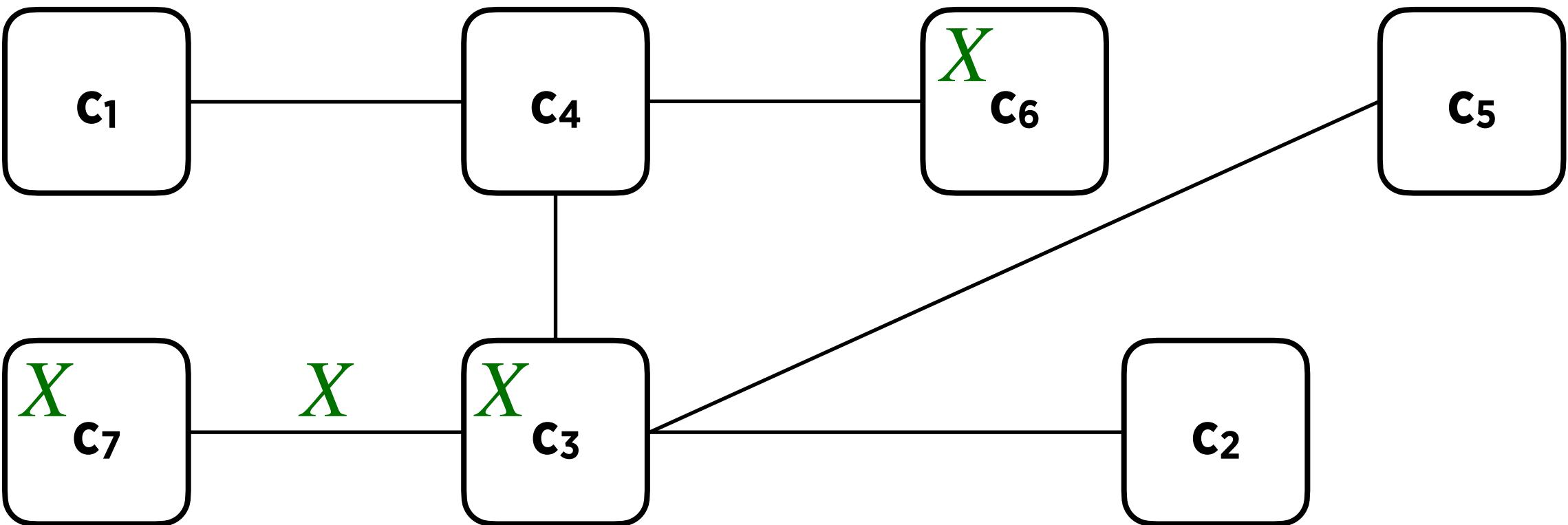
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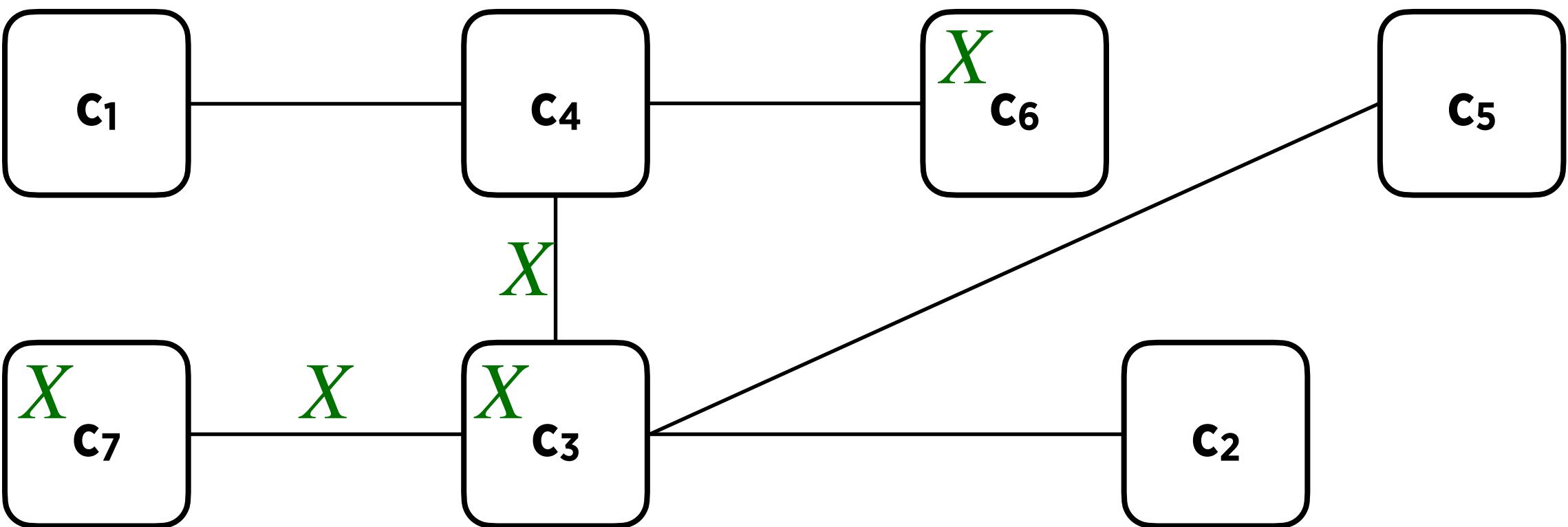
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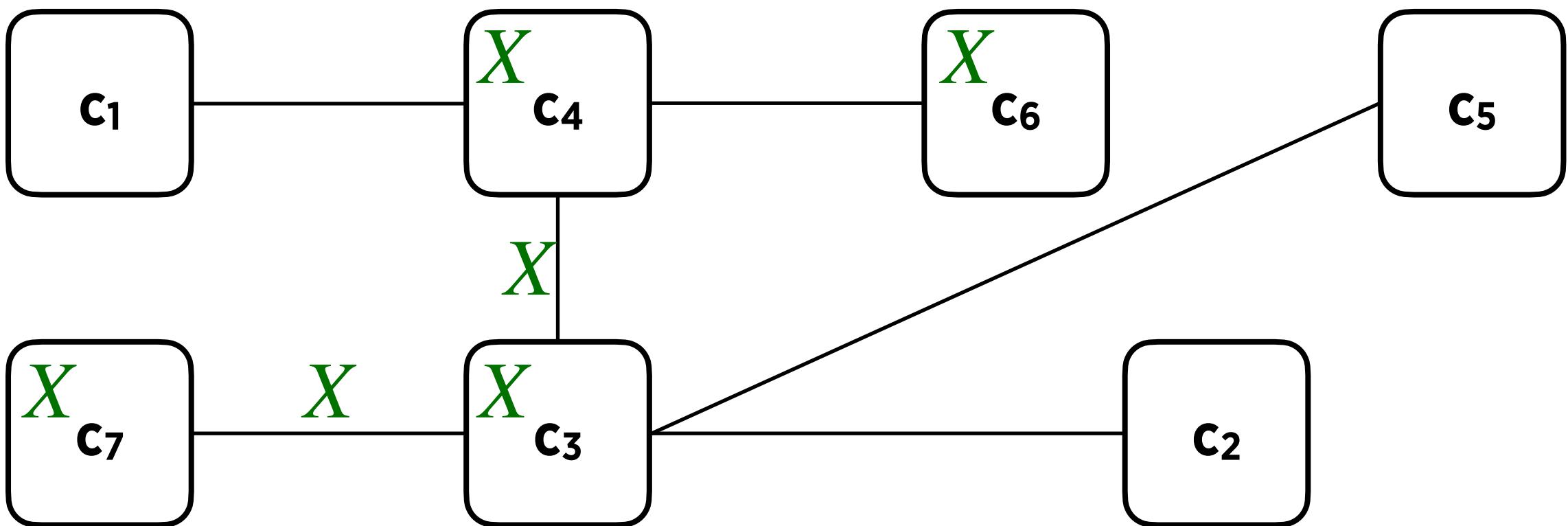
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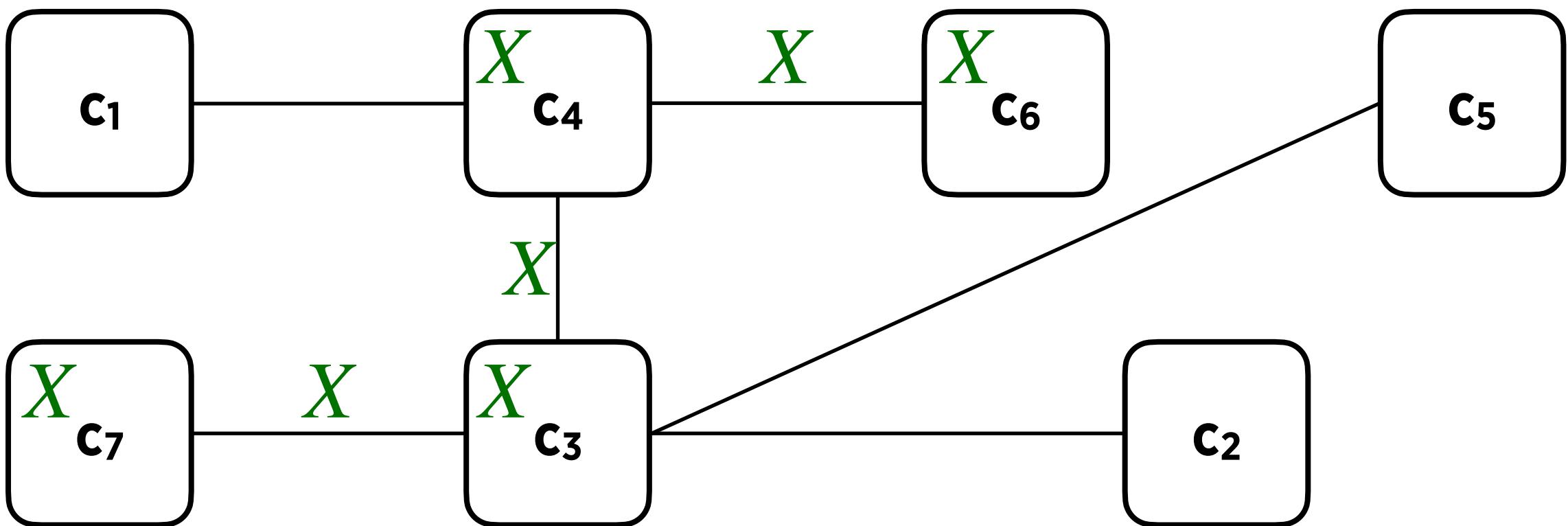
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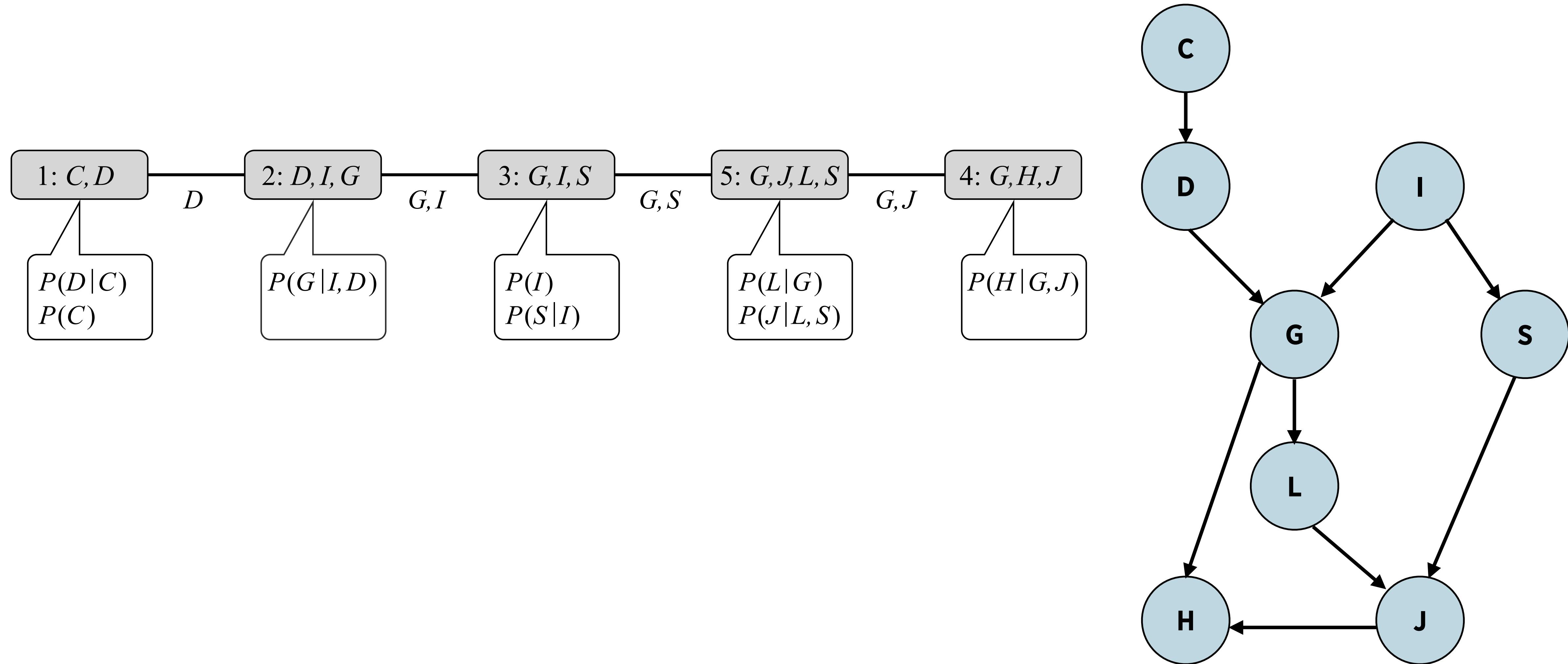


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# More complex clique tree



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- In this case, computation is a variant of variable elimination
- Resulting beliefs are guaranteed to be correct marginals

# Pgmpy

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Installation

Requirements

Contributing to pgmpy

License

**BASE STRUCTURES**

Directed Acyclic Graph (DAG)

Partial Directed Acyclic Graph (PDAG)

**MODELS**

Bayesian Network

Dynamic Bayesian Network (DBN)

Structural Equation Models (SEM)

Naive Bayes

NoisyOr Model

Markov Network

Junction Tree

Cluster Graph

Factor Graph

Markov Chain

**PARAMETERIZATION**

Discrete

Discretizing Methods

**EXACT INFERENCE**

Variable Elimination

Elimination Ordering

Belief Propagation

Causal Inference

MPLP

» Installation

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## Installation

pgmpy requires Python 3.7+. pgmpy is hosted on both pypi and anaconda. For installation through pypi, use the command:

```
pip install pgmpy
```

For installation through anaconda, use the command:

```
conda install -c ankurrankan pgmpy
```

For installing the latest *dev* branch from github, use the command:

```
pip install git+https://github.com/pgmpy/pgmpy.git@dev
```

## Requirements

If installing manually, the following non-optional dependencies needs to be installed:

- Python 3.7+
- numpy
- scipy
- scikit-learn
- pandas
- pyparsing
- pytorch
- statsmodels
- tqdm
- joblib

◁ ▷ ⌂ 🔒 pgmpy.org/models/bayesianetwork.html

Bayesian Network

- Dynamic Bayesian Network (DBN)
- Structural Equation Models (SEM)
- Naive Bayes
- NoisyOr Model
- Markov Network
- Junction Tree
- Cluster Graph
- Factor Graph
- Markov Chain

**PARAMETERIZATION**

- Discrete
- Discretizing Methods

**EXACT INFERENCE**

- Variable Elimination
- Elimination Ordering
- Belief Propagation
- Causal Inference
- MPLP

Dynamic Bayesian Network Inference

Model Testing

**APPROXIMATE INFERENCE**

- Approximate Inference Using Sampling
- Bayesian Model Sampling
- Gibbs Sampling

**PARAMETER ESTIMATION**

- Maximum Likelihood Estimator

» Bayesian Network

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# Bayesian Network

`class pgmpy.models.BayesianNetwork(ebunch=None, latents={})` [\[source\]](#)

Base class for Bayesian Models.

`| add_cpds(*cpds)` [\[source\]](#)

Add CPD (Conditional Probability Distribution) to the Bayesian Model.

**Parameters:** cpds (`list, set, tuple (array-like)`) – List of CPDs which will be associated with the model

**Examples**

```
>>> from pgmpy.models import BayesianNetwork
>>> from pgmpy.factors.discrete.CPD import TabularCPD
>>> student = BayesianNetwork([('diff', 'grades'), ('intel', 'grades')])
>>> grades_cpd = TabularCPD('grades', 3, [[0.1,0.1,0.1,0.1,0.1,0.1],
...                                         [0.1,0.1,0.1,0.1,0.1,0.1],
...                                         [0.8,0.8,0.8,0.8,0.8,0.8]],
...                                         evidence=['diff', 'intel'], evidence_card=[2, 3])
>>> student.add_cpds(grades_cpd)
```

diff:	easy			hard		
intel:	dumb	avg	smart	dumb	avg	smart
gradeA	0.1	0.1	0.1	0.1	0.1	0.1
gradeB	0.1	0.1	0.1	0.1	0.1	0.1
gradeC	0.8	0.8	0.8	0.8	0.8	0.8

`| add_edge(u, v, **kwargs)` [\[source\]](#)

Add an edge between u and v.

Variable Elimination

- Elimination Ordering
- Belief Propagation
- Causal Inference
- MPLP
- Dynamic Bayesian Network Inference
- Model Testing

APPROXIMATE INFERENCE

- Approximate Inference Using Sampling
- Bayesian Model Sampling
- Gibbs Sampling

PARAMETER ESTIMATION

- Maximum Likelihood Estimator
- Bayesian Estimator
- Expectation Maximization (EM)
- Structural Equation Model Estimators

STRUCTURE LEARNING

- PC (Constraint-Based Estimator)
- Conditional Independence Tests for PC algorithm
- Hill Climb Search
- Structure Score
- Tree Search
- Mmhc Estimator
- Exhaustive Search

MODEL TESTING

- Metrics for testing models

» Variable Elimination

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## Variable Elimination

`class pgmpy.inference.ExactInference.VariableElimination(model) [source]`

`induced_graph(elimination_order) [source]`

Returns the induced graph formed by running Variable Elimination on the network.

**Parameters:** `elimination_order (list, array like)` – List of variables in the order in which they are to be eliminated.

**Examples**

```
>>> import numpy as np
>>> import pandas as pd
>>> from pgmpy.models import BayesianNetwork
>>> from pgmpy.inference import VariableElimination
>>> values = pd.DataFrame(np.random.randint(low=0, high=2, size=(1000, 5)),
...                         columns=['A', 'B', 'C', 'D', 'E'])
>>> model = BayesianNetwork([('A', 'B'), ('C', 'B'), ('C', 'D'), ('B', 'E')])
>>> model.fit(values)
>>> inference = VariableElimination(model)
>>> inference.induced_graph(['C', 'D', 'A', 'B', 'E'])
```

`induced_width(elimination_order) [source]`

Returns the width (integer) of the induced graph formed by running Variable Elimination on the network. The width is defined as the number of nodes in the largest clique in the graph minus 1.

**Parameters:** `elimination_order (list, array like)` – List of variables in the order in which they are to be eliminated.

**Examples**

```
>>> import numpy as np
>>> import pandas as pd
```