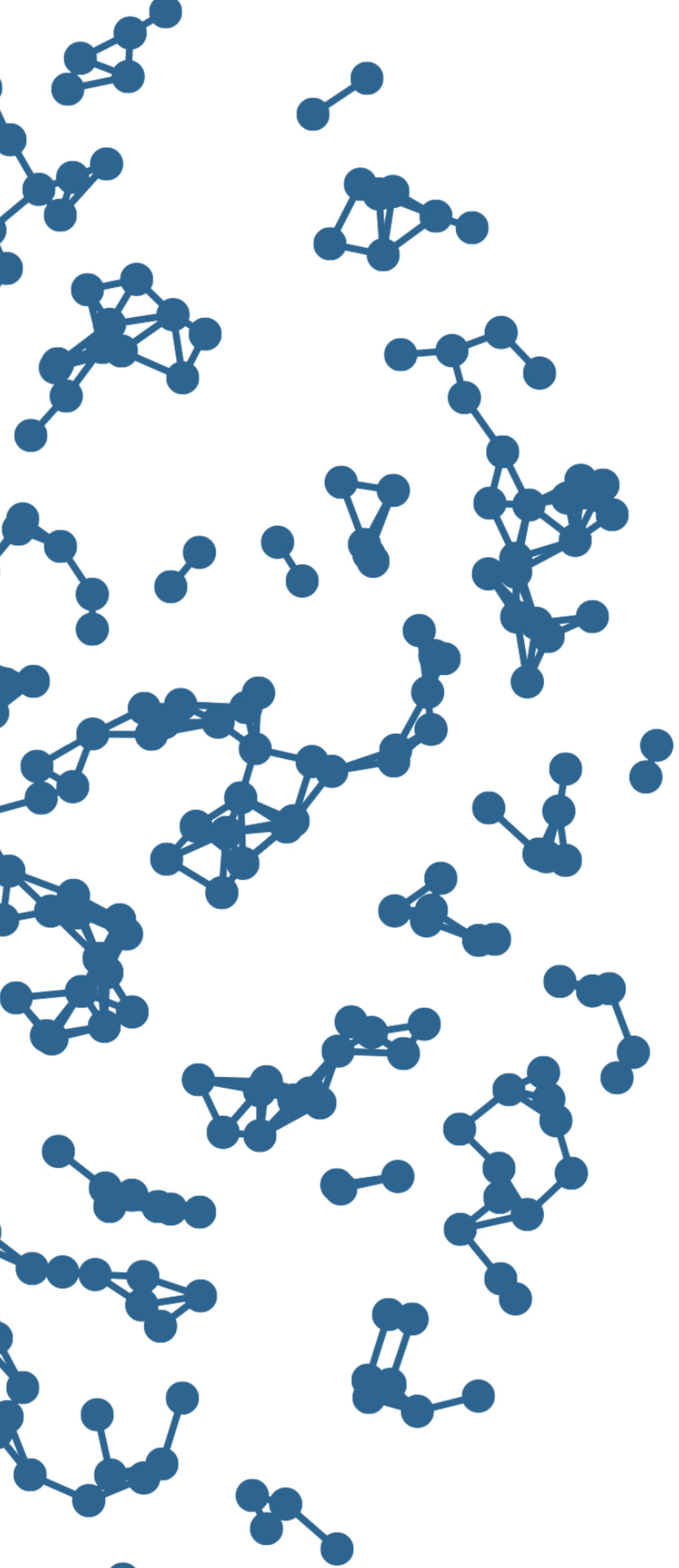
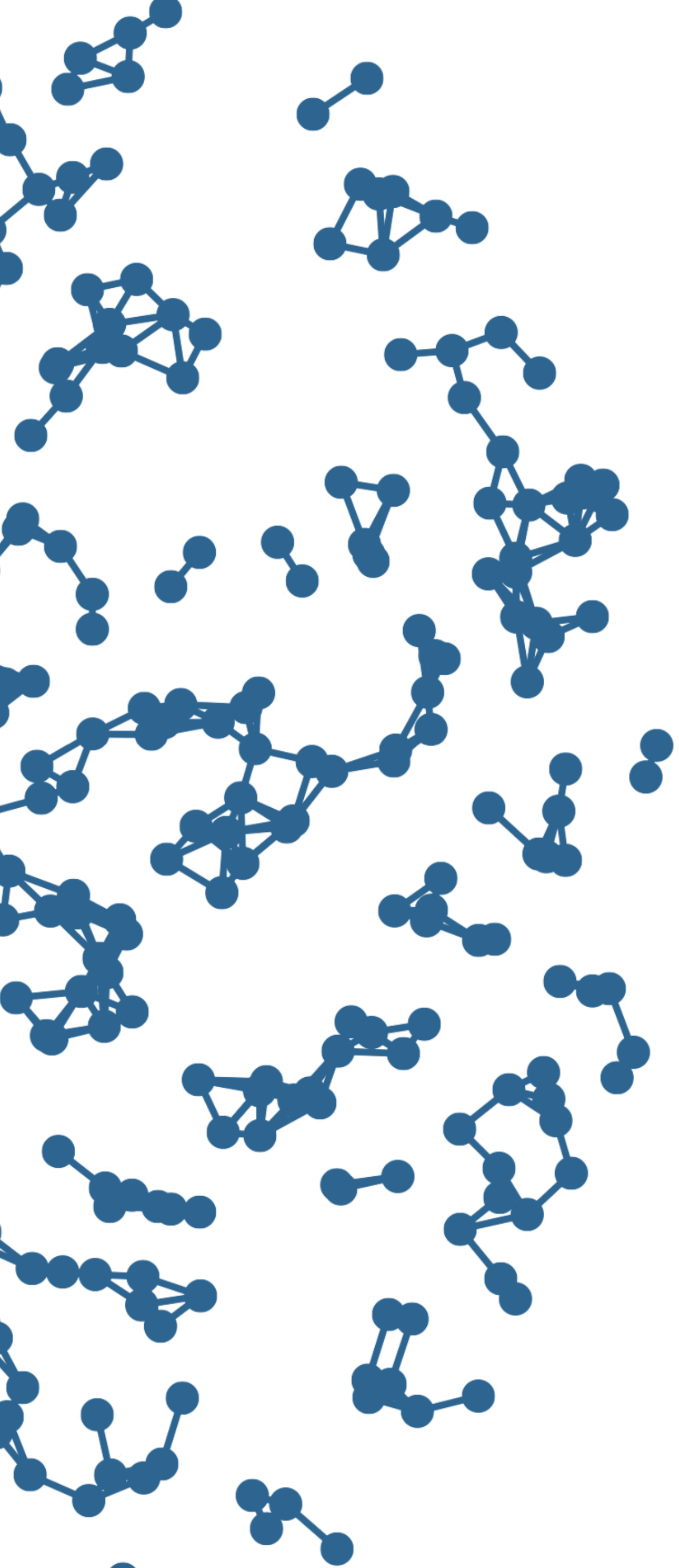


STOCHASTIC SPREADING ON COMPLEX NETWORKS

Gerrit Großmann

12.12.2022



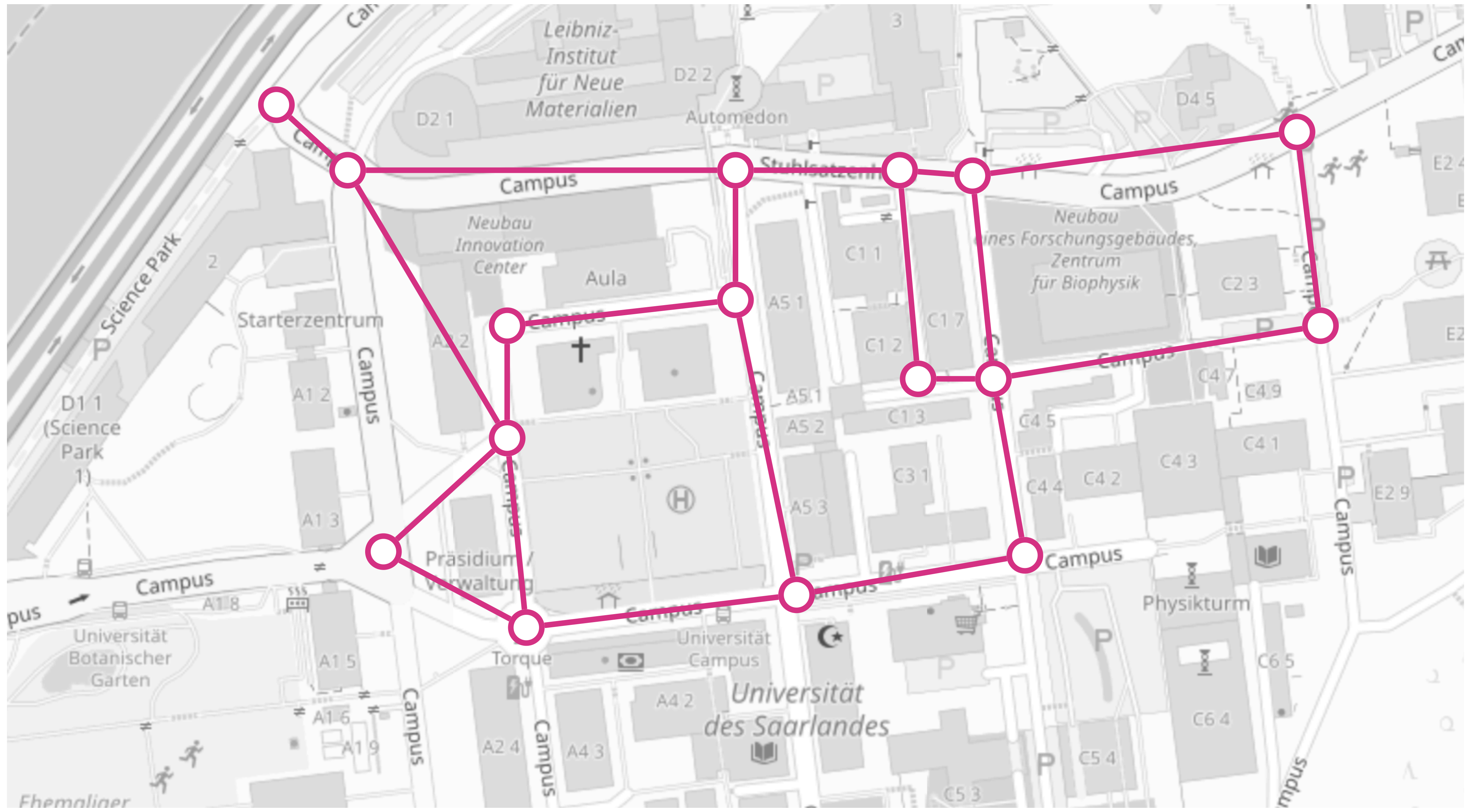
Prologue

NETWORKS ARE EVERYWHERE

In many ways, graphs are the main modality of data we receive from nature.

- Petar Veličković

OpenStreetMap



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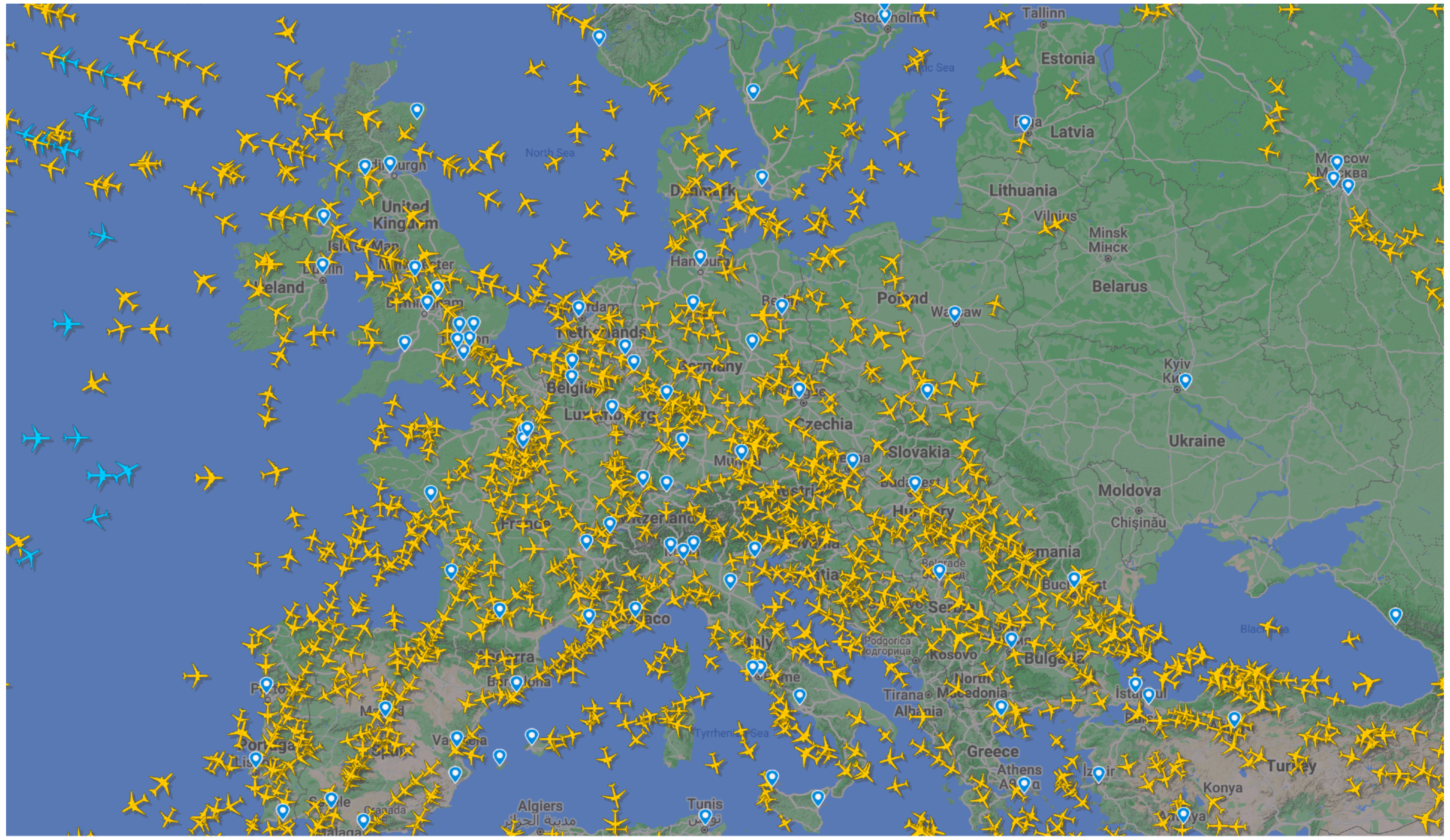

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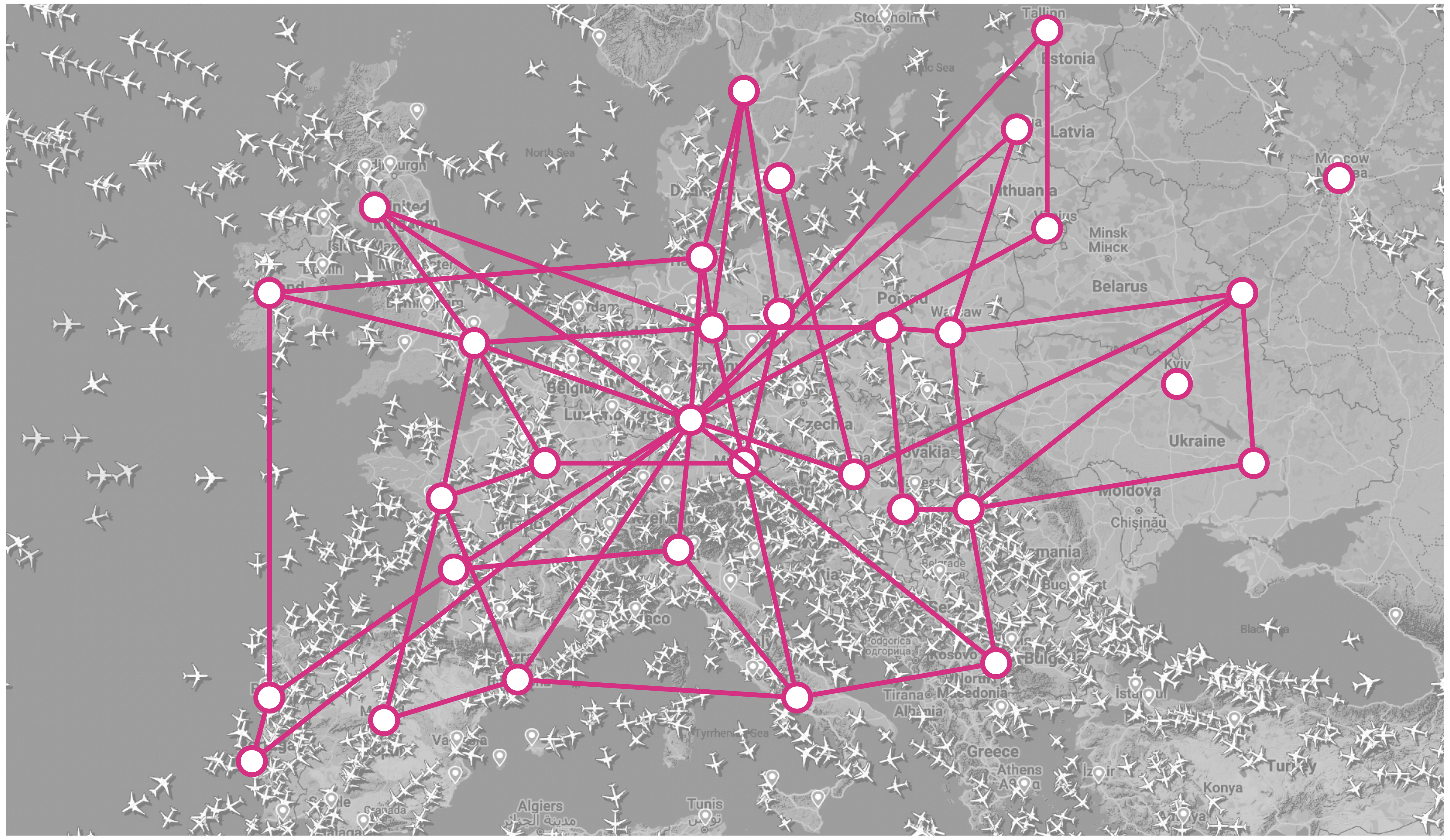
flightradar24.com/49.73,7.2/5



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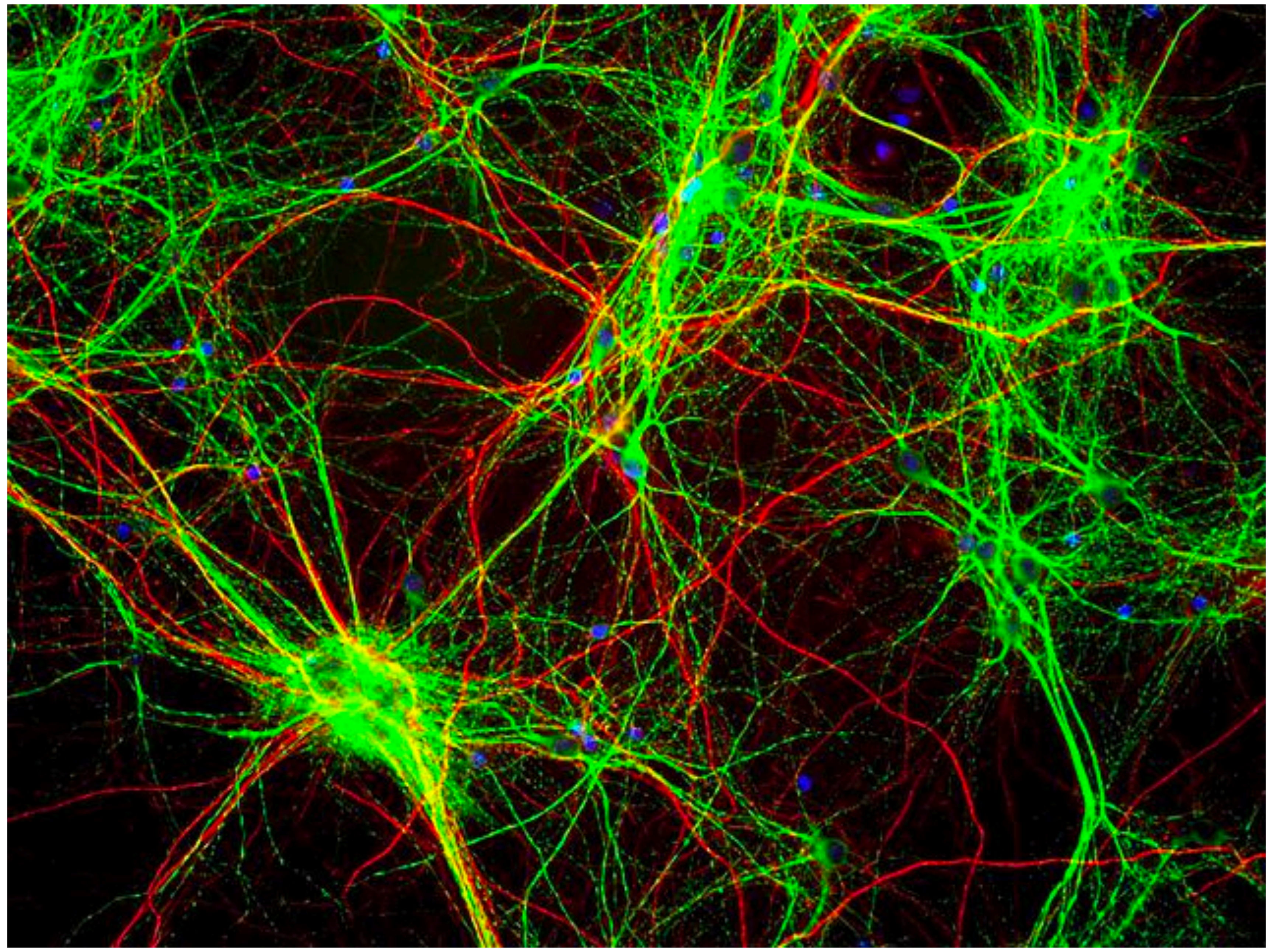

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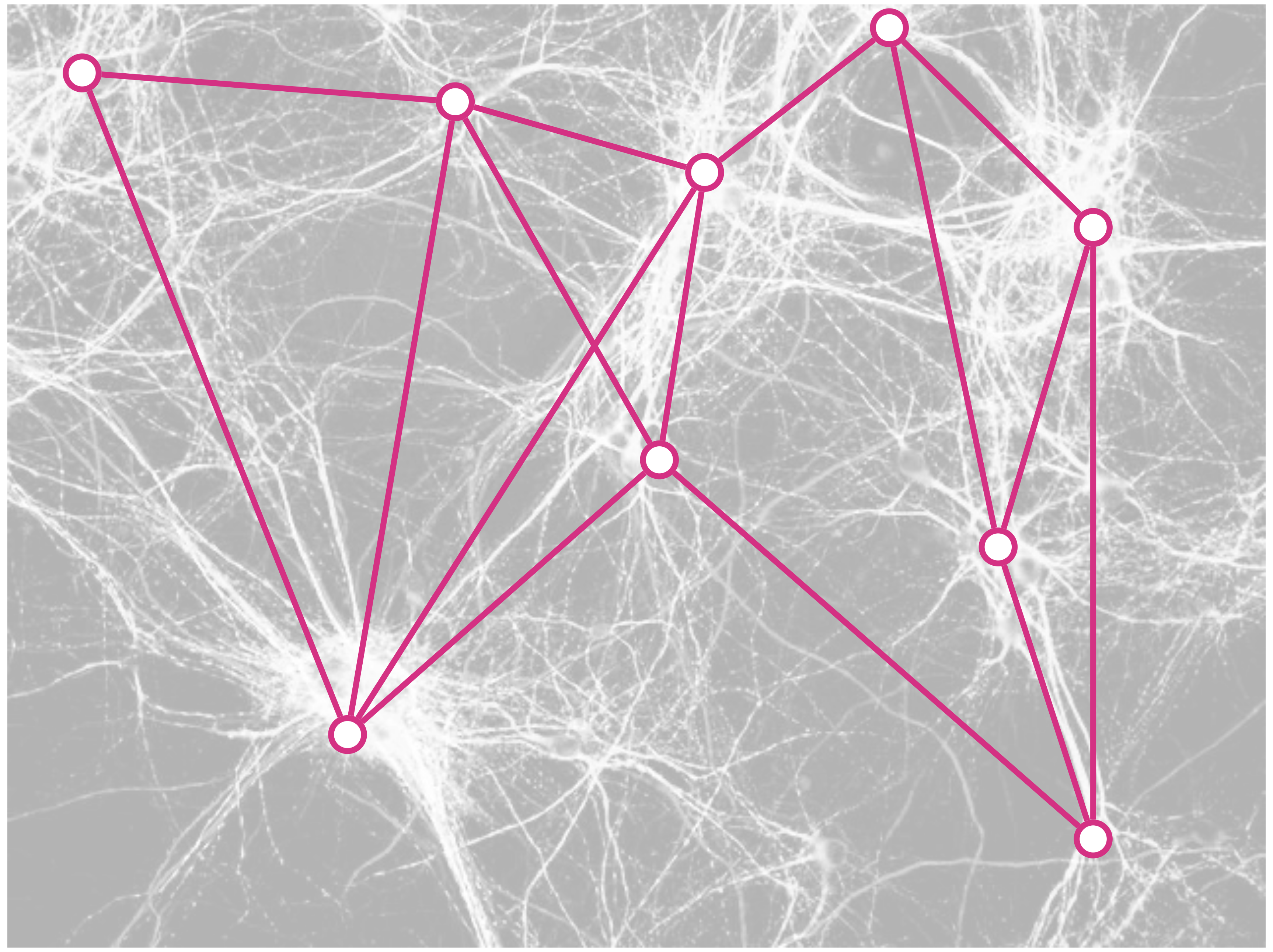
https://commons.wikimedia.org/w/index.php?search=Gerry+Shaw+neuron&title=Special:MediaSearch&go=Go&type=image



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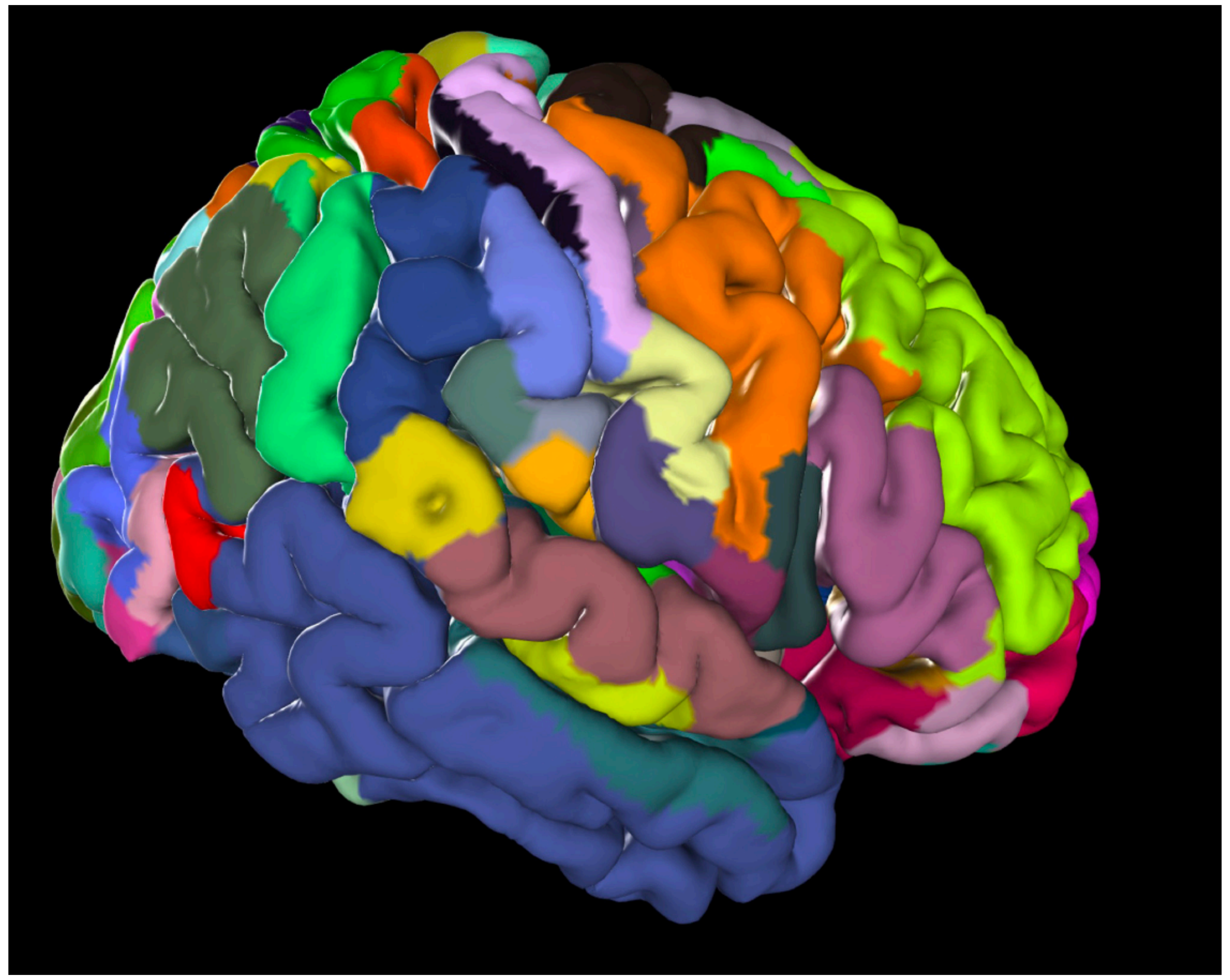

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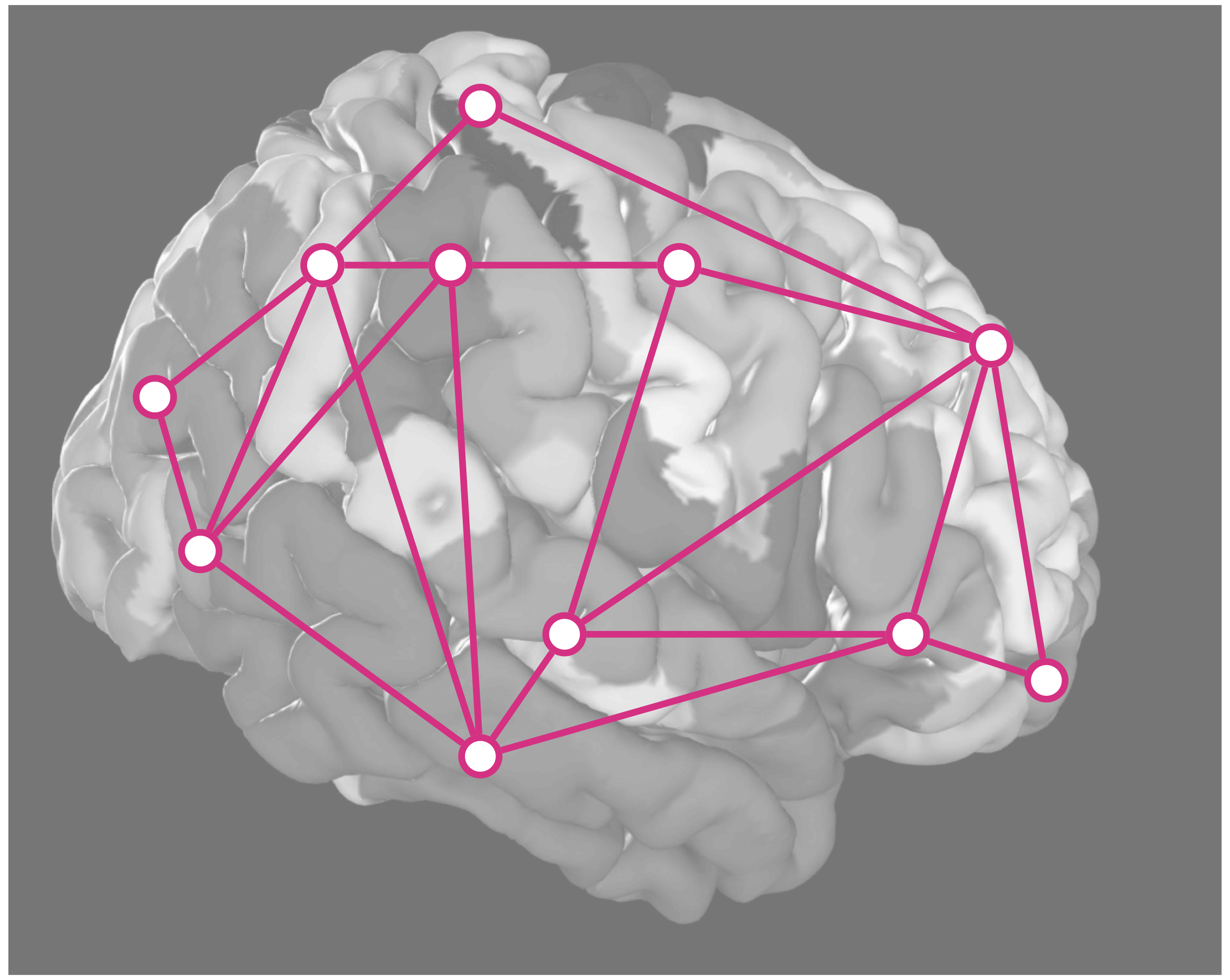
fz-juelich.de/de/aktuelles/news/pressemitteilungen/2020/2020-07-31-julich-brain-atlas



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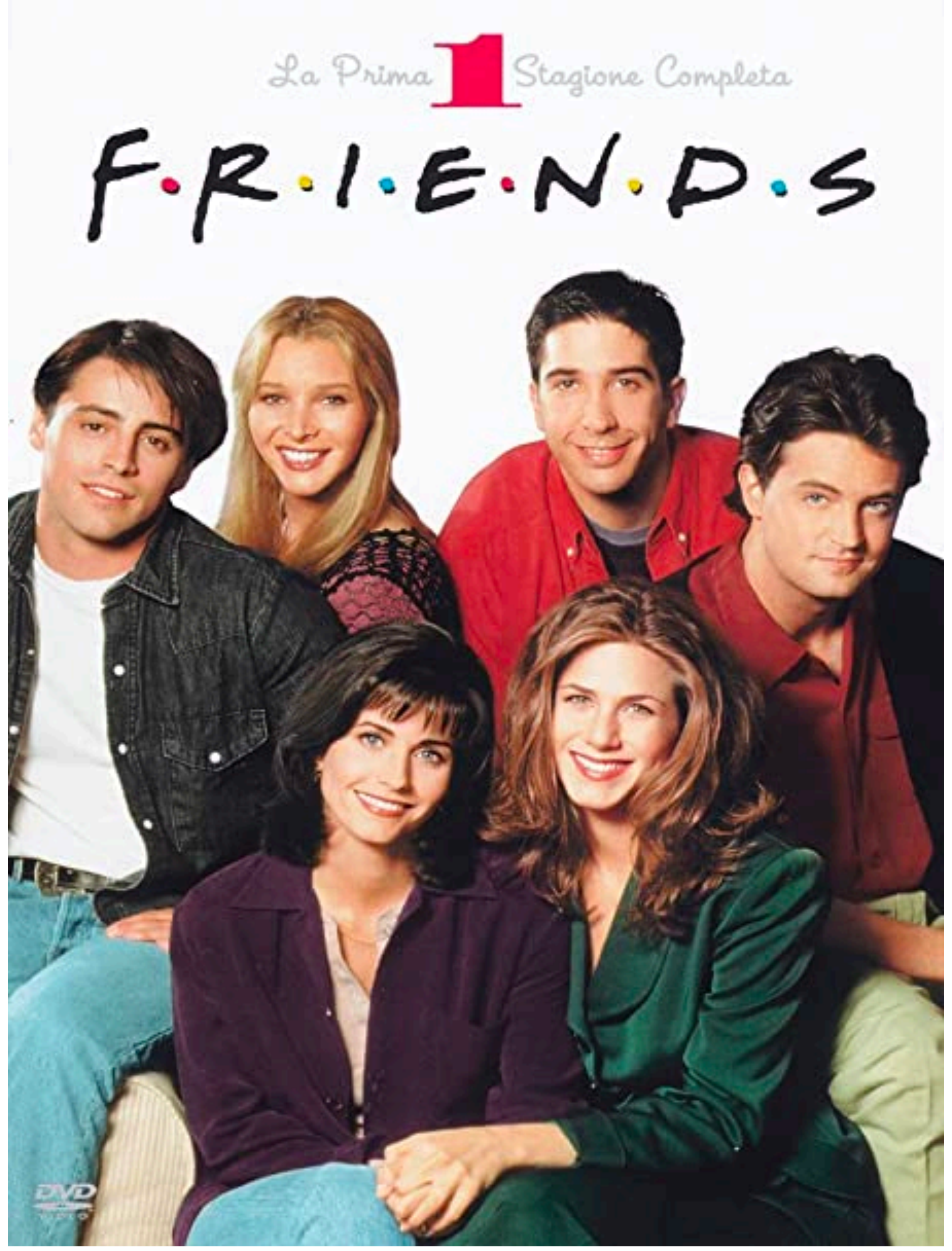

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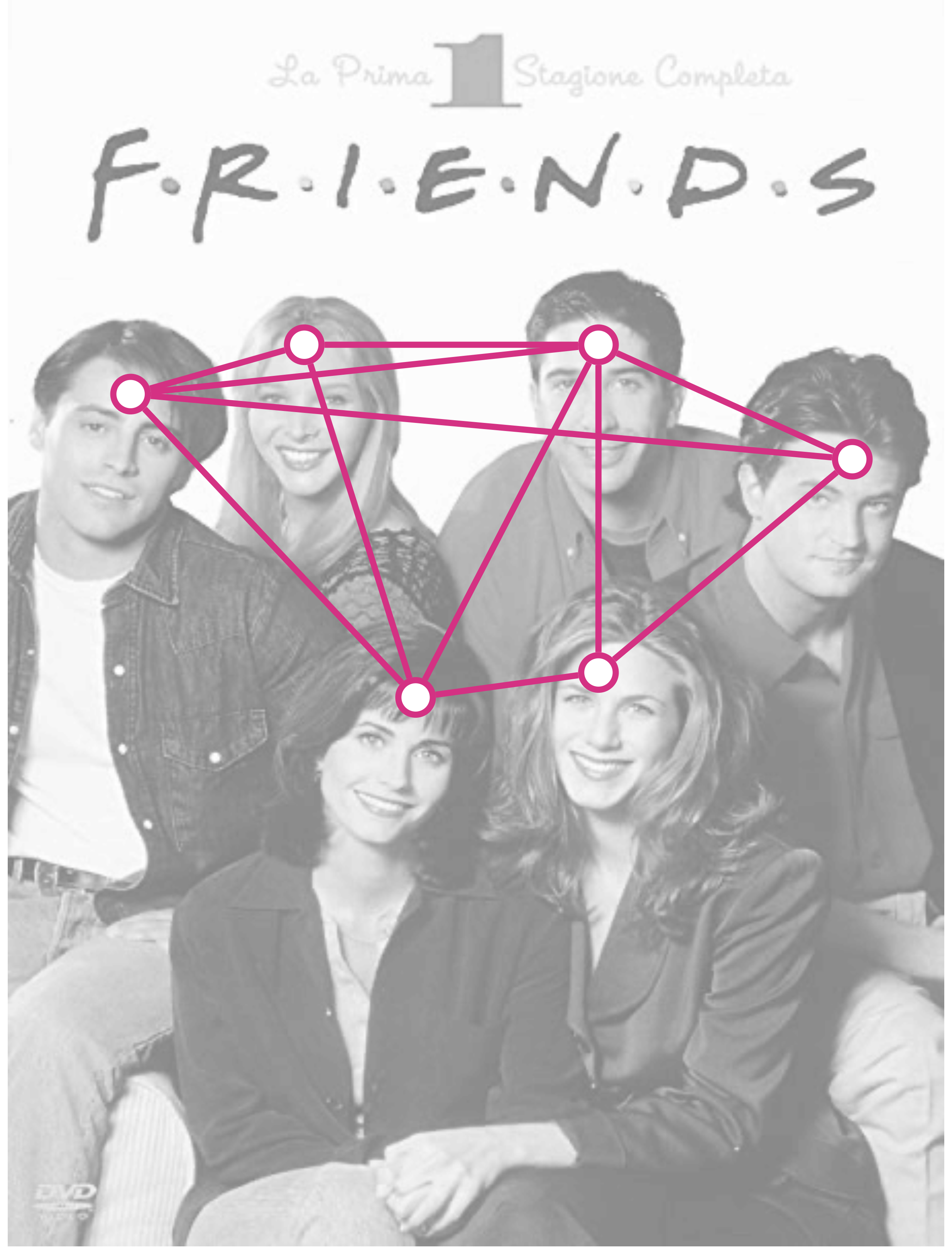

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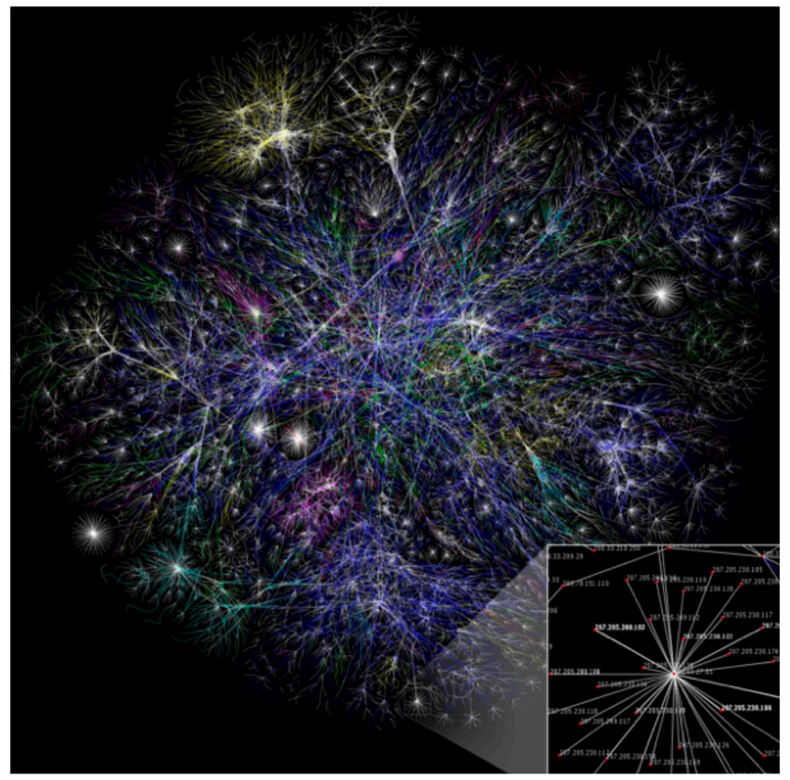

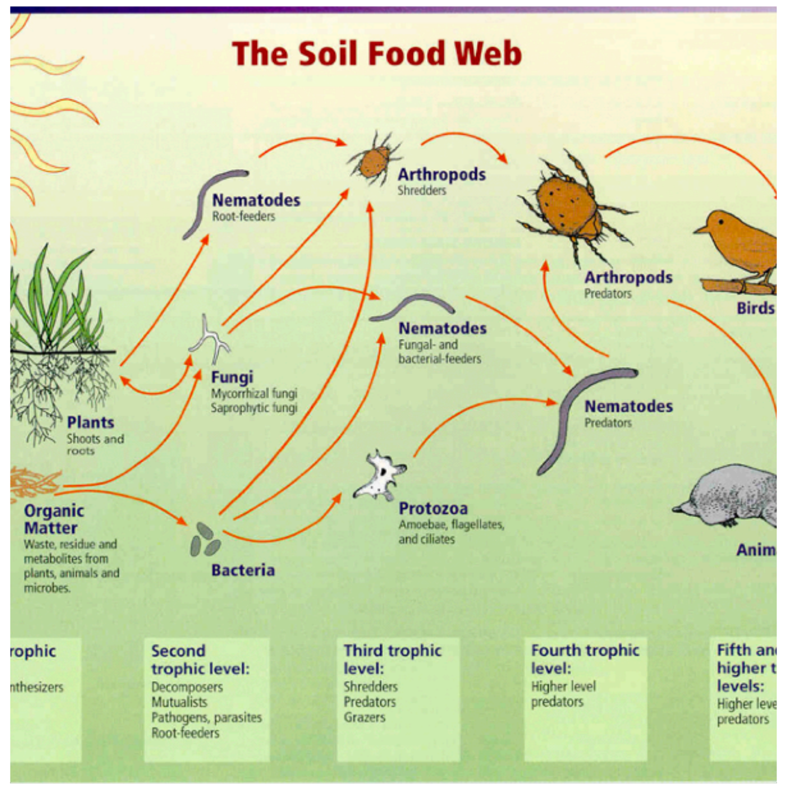

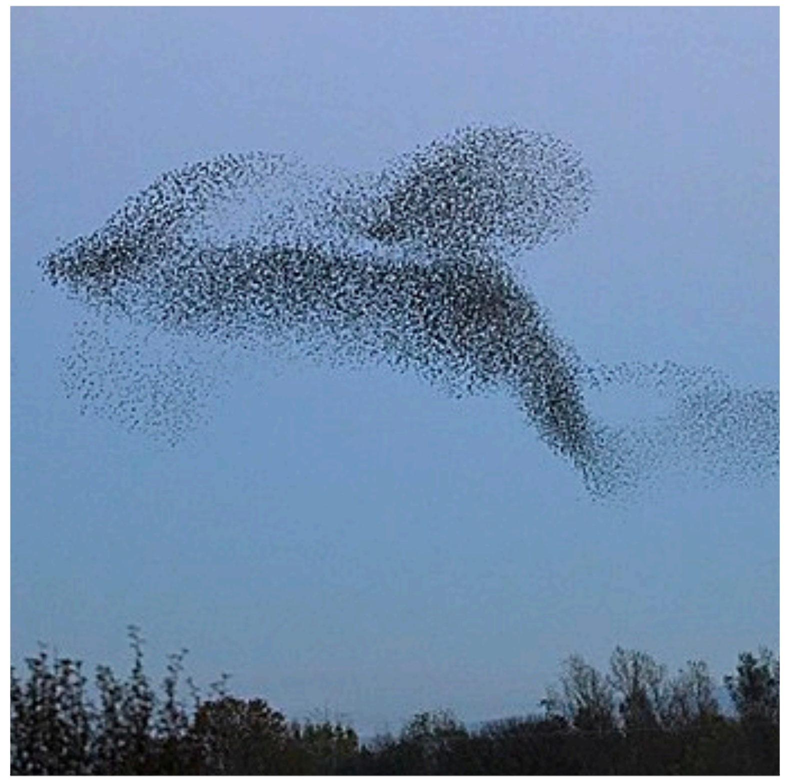

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commons.wikimedia.org/wiki/File:Philippine-stock-market-board.jpg
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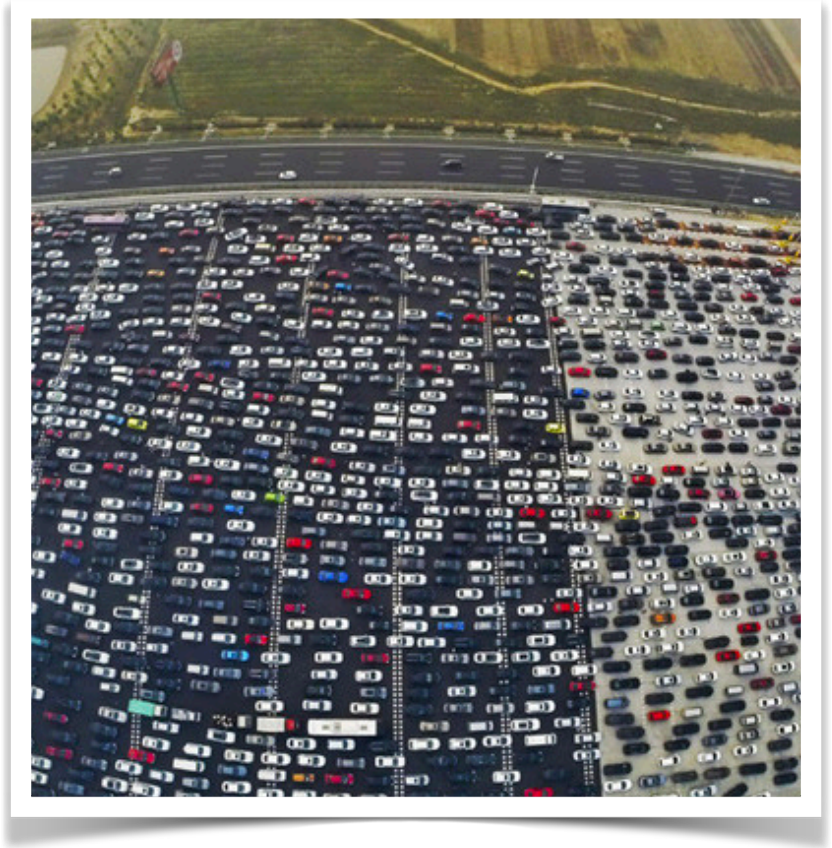

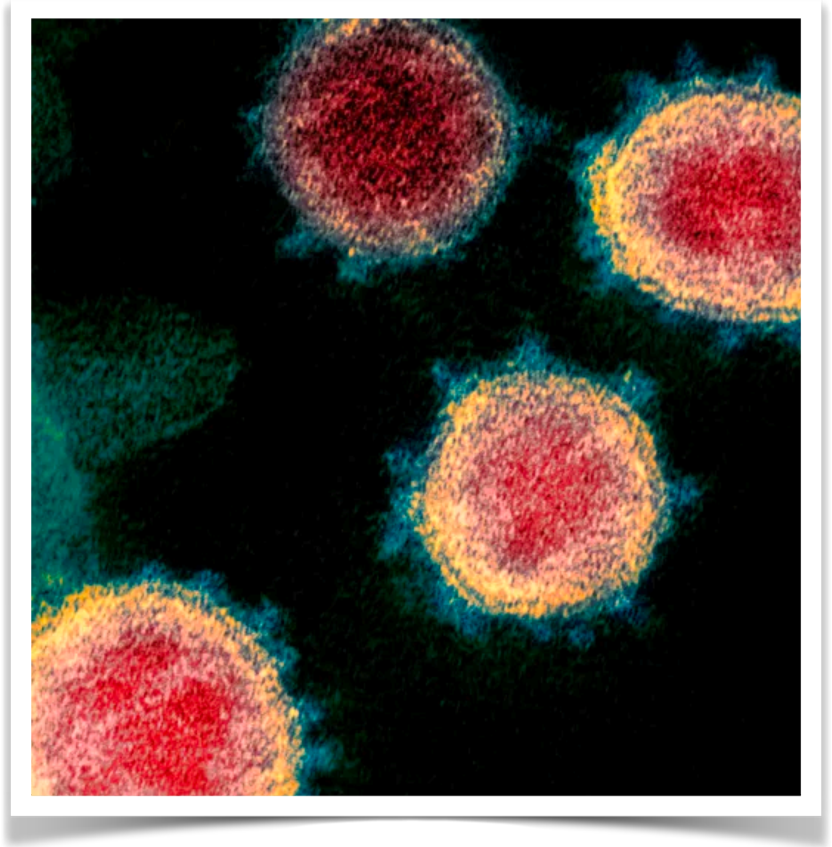

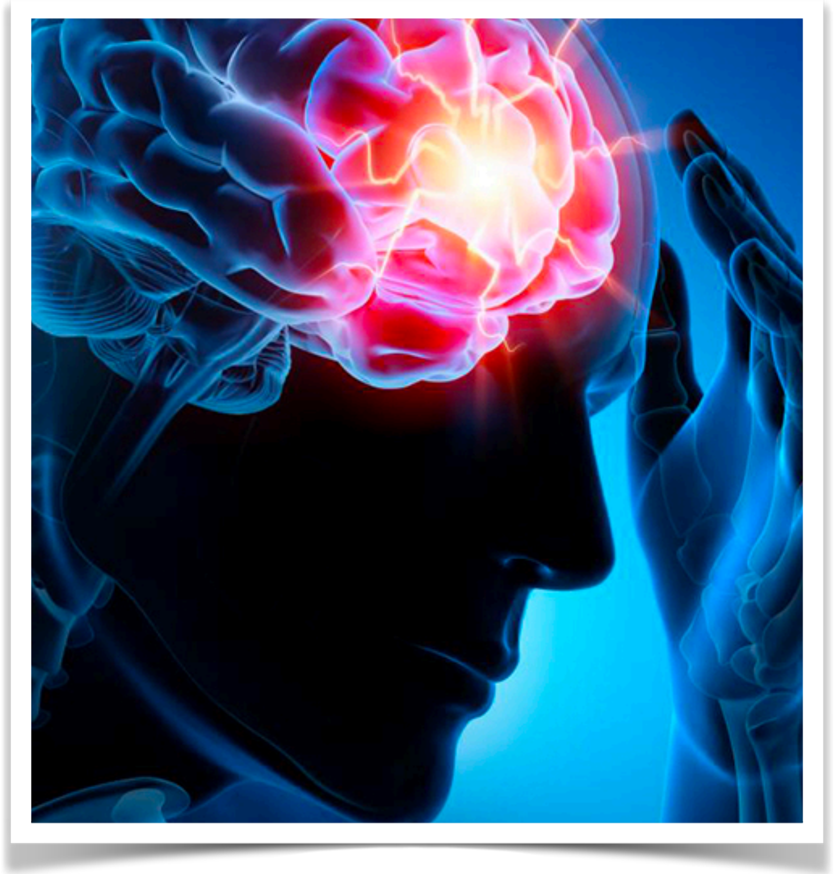

Pope Francis Shocks World, Endorses Donald Trump for President, Releases Statement

TOPICS: Pope Francis Endorses Donald Trump

Wrong again. WTOE5

Facebook engagements: 961,300

When there is a network, things will spread.

nymag.com/intelligencer/2019/07/manhattan-power-outage.html
spiegel.de/wissenschaft/medizin/coronavirus-grosse-antikoerper-studie-soll-immunitaet-der-deutschen-feststellen-a-c8c64a33-5c0f-4630-bd73-48c17c1bad23
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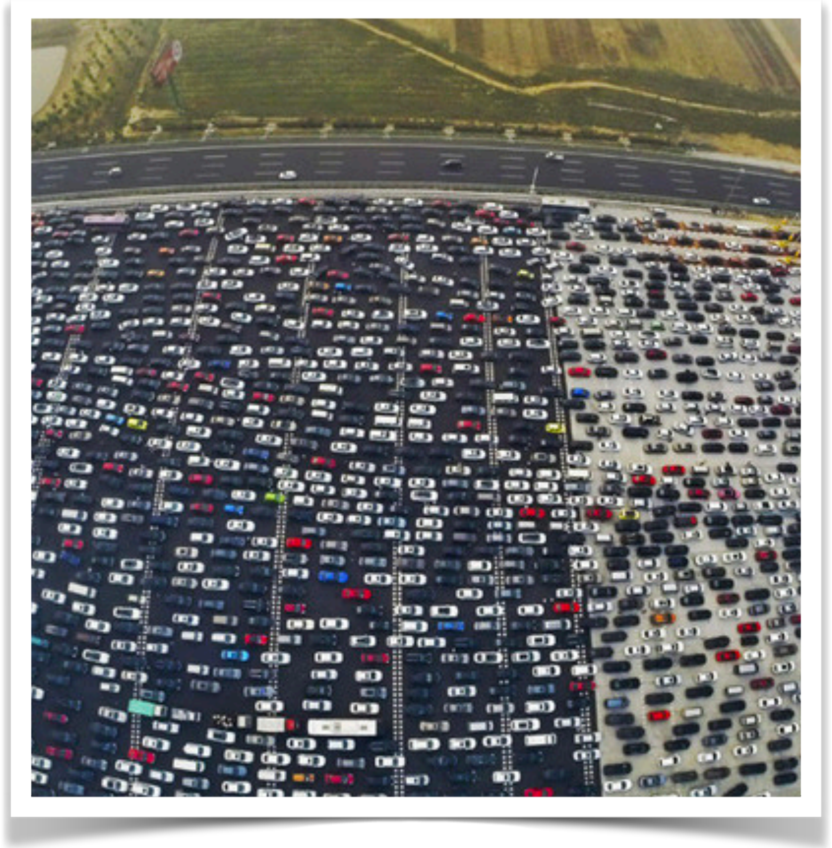

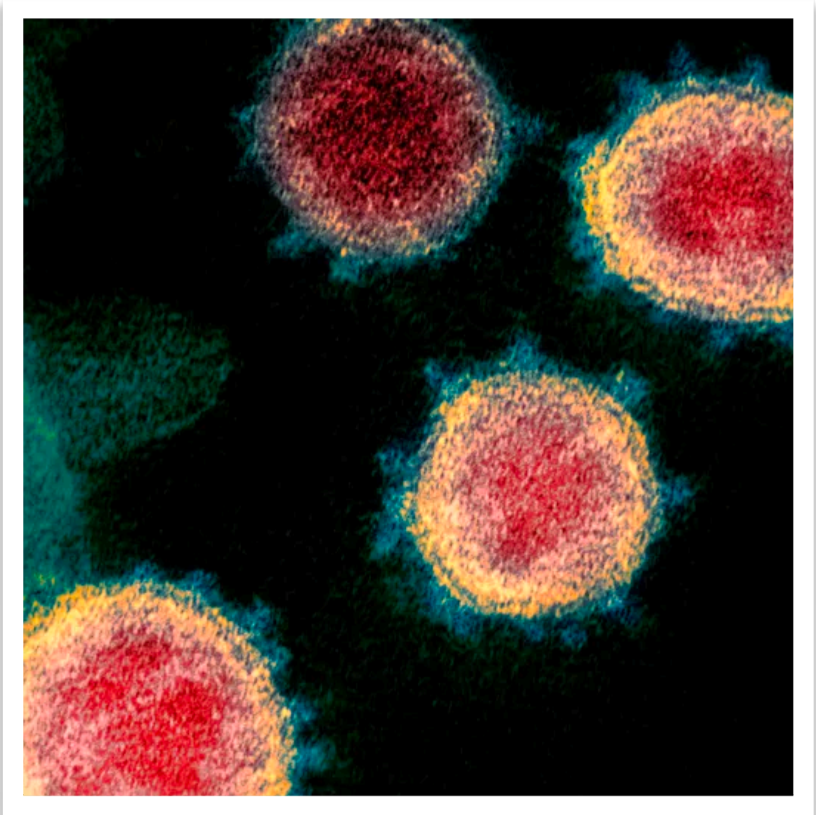

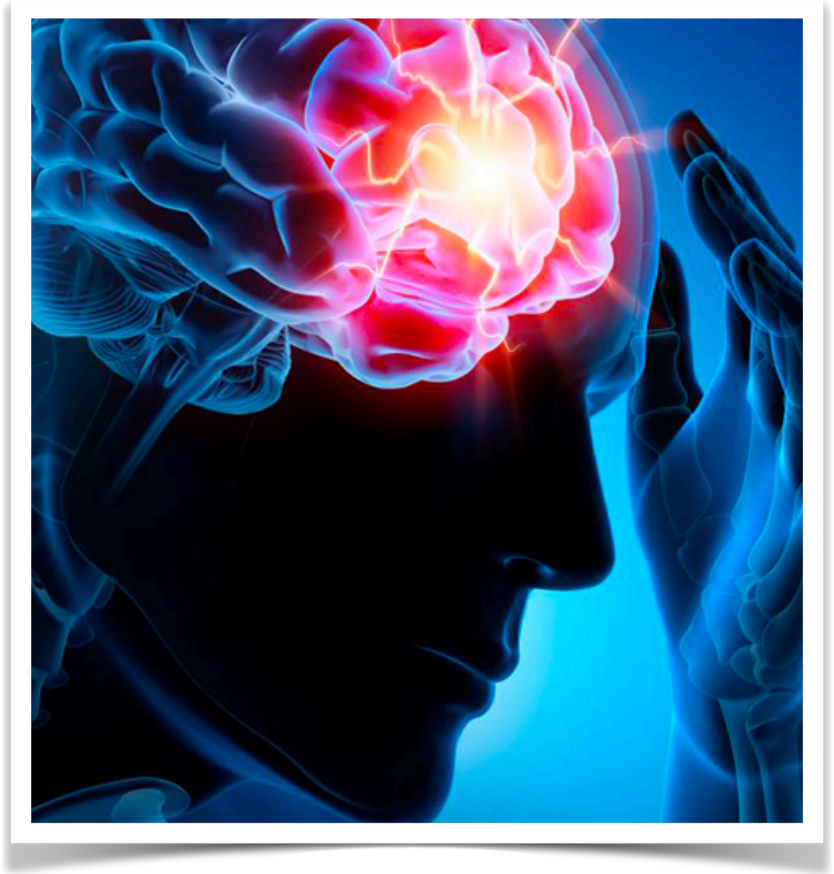

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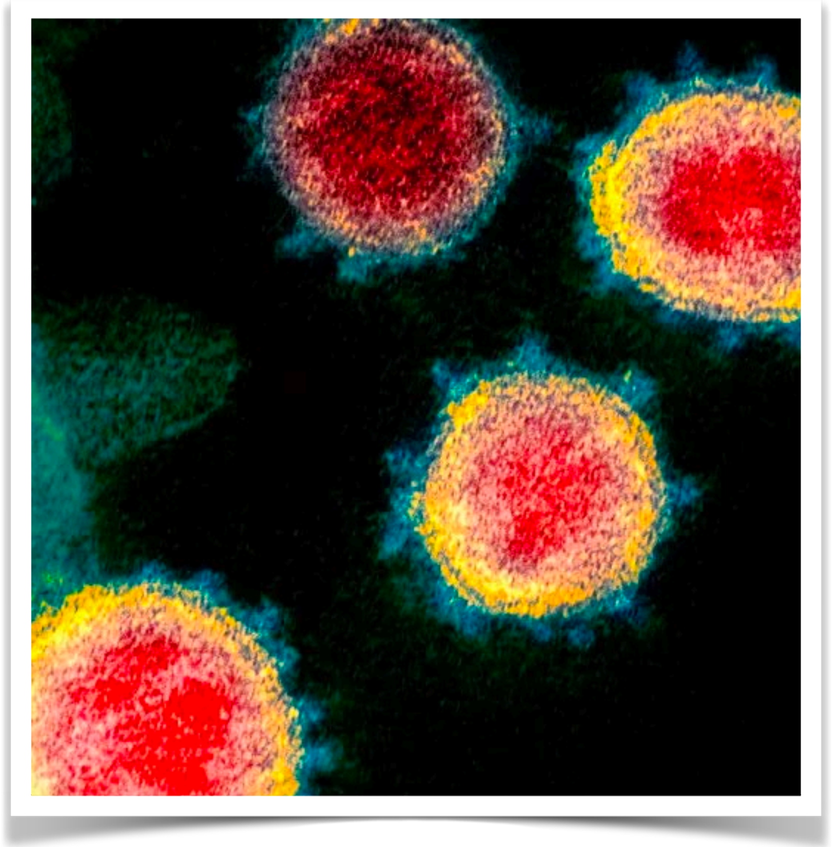
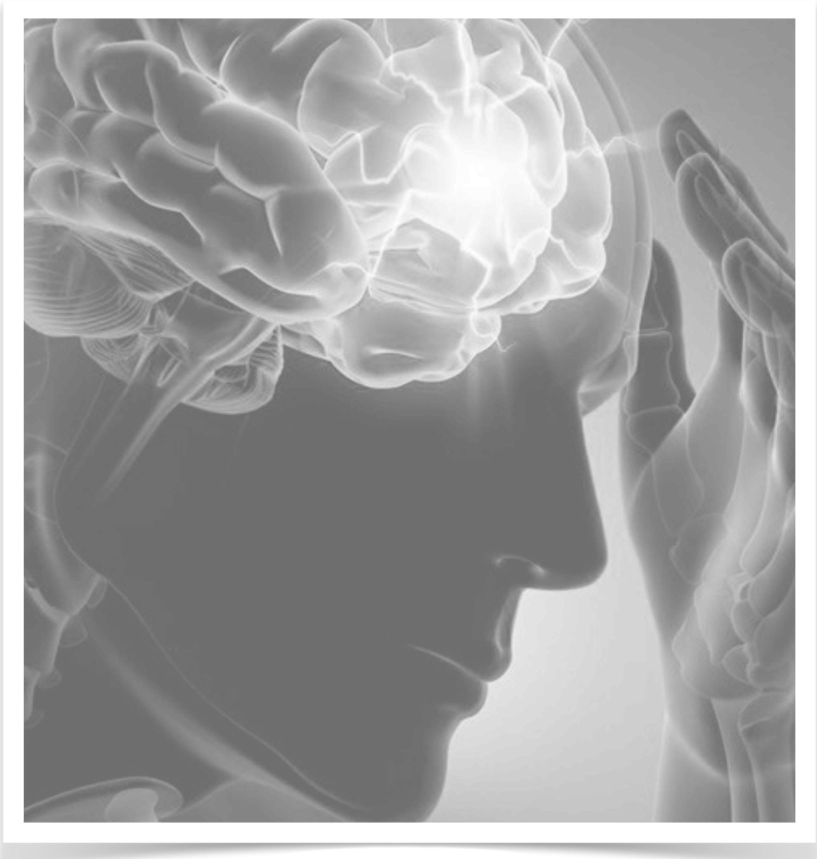
Goal: Build a mathematical model of information diffusion.





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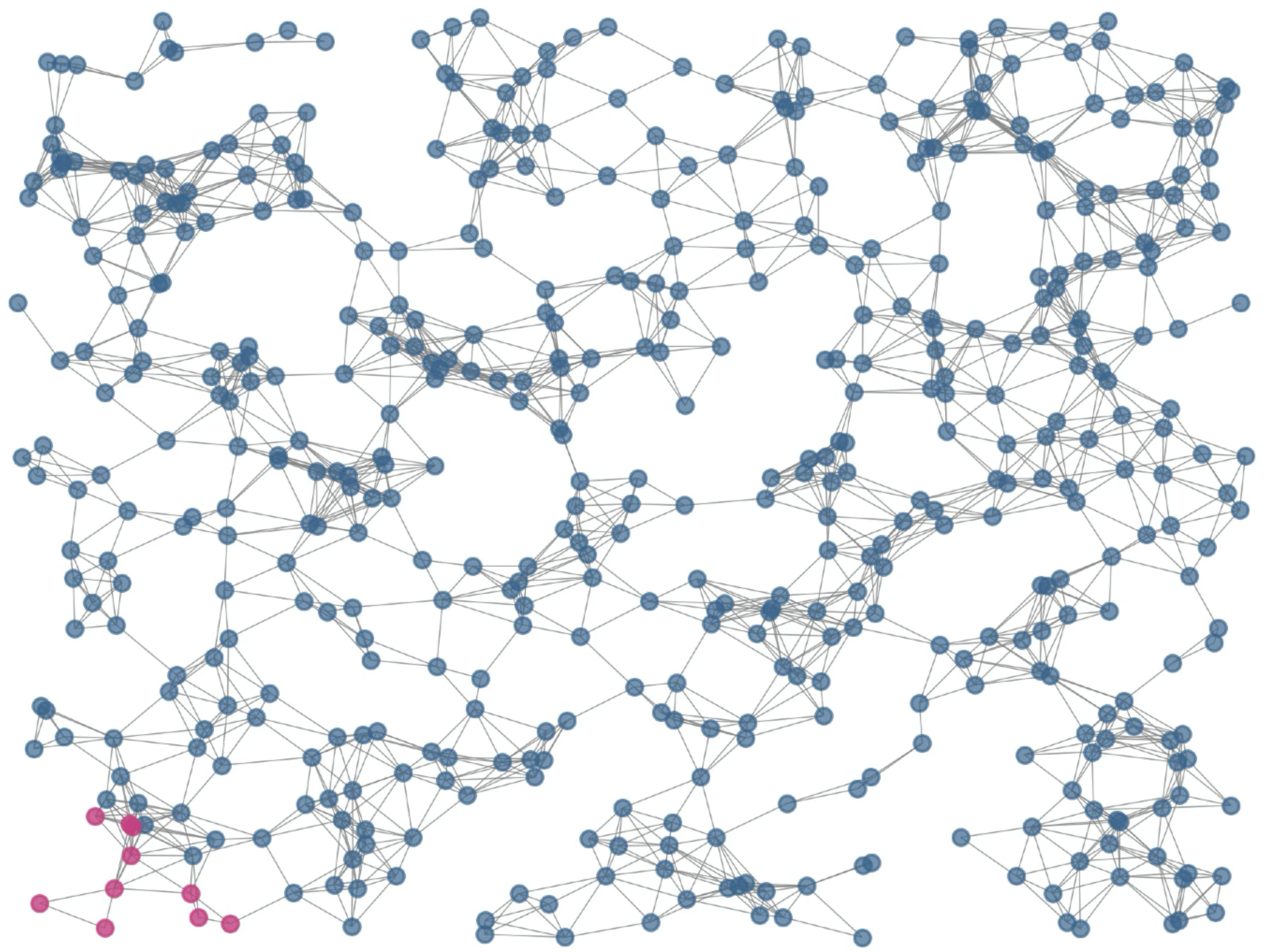
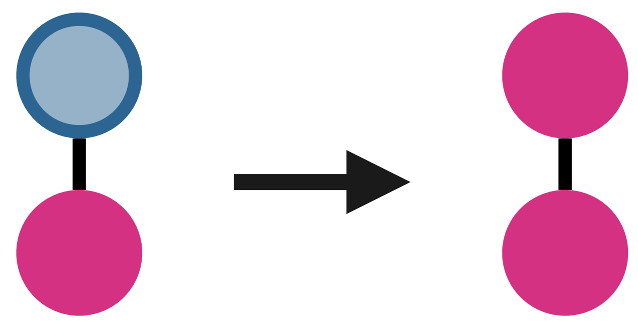
Everything that spreads is an epidemic.

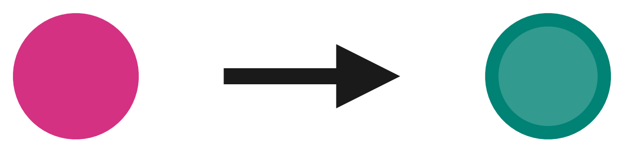
SIR



- Nodes are **susceptible**, **infected**, **recovered**.

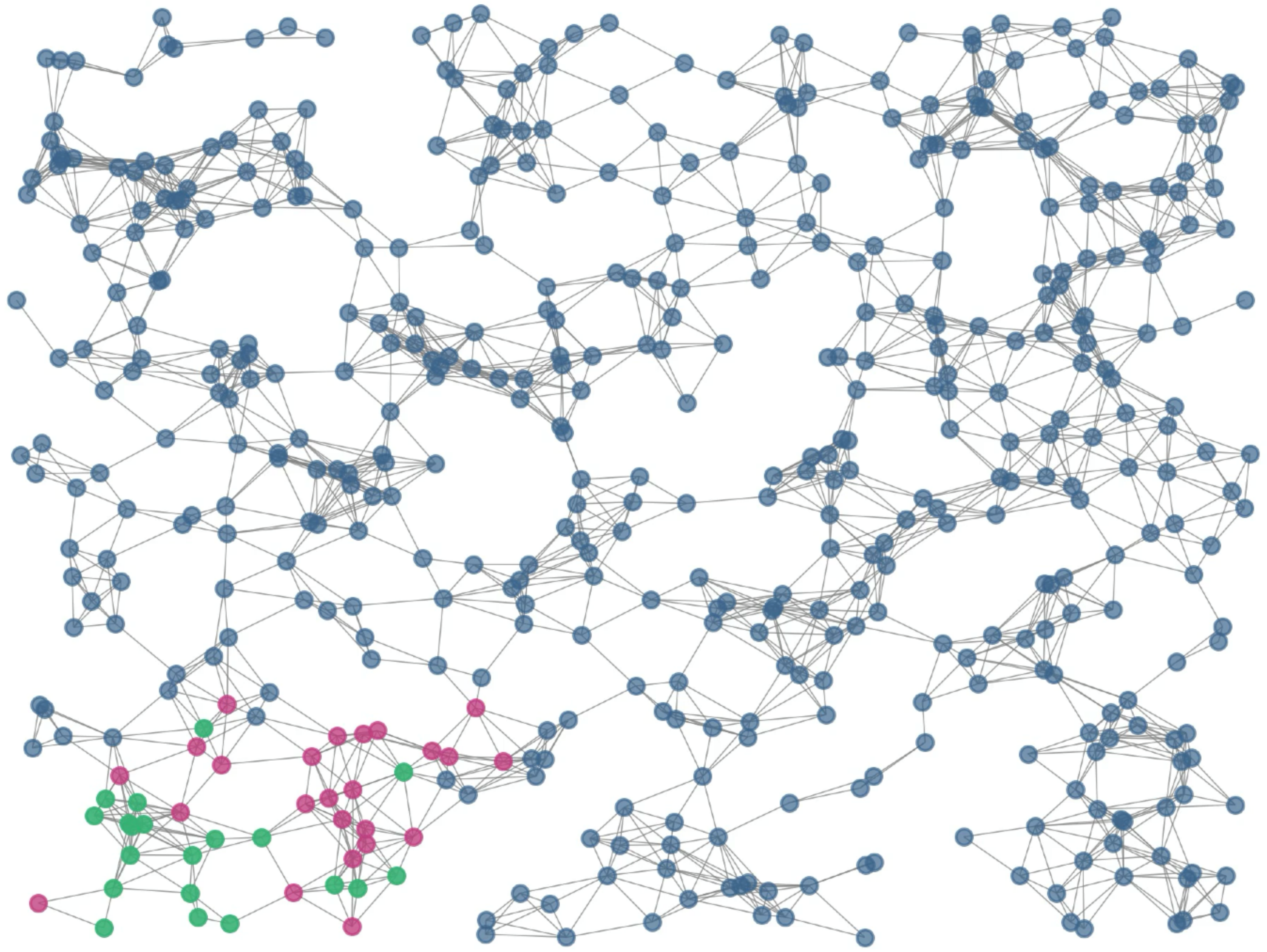


- **Infected** nodes infect **susceptible** neighbors.



- **Infected** nodes recover (gain immunity).

SIR



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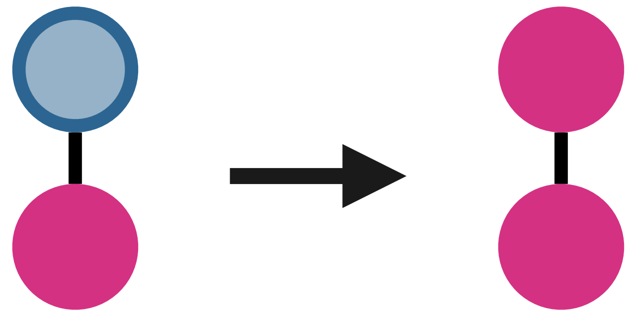

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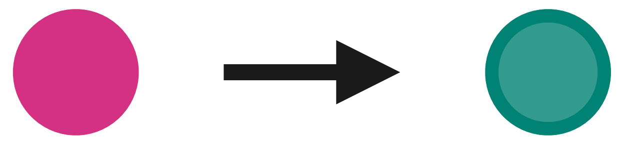

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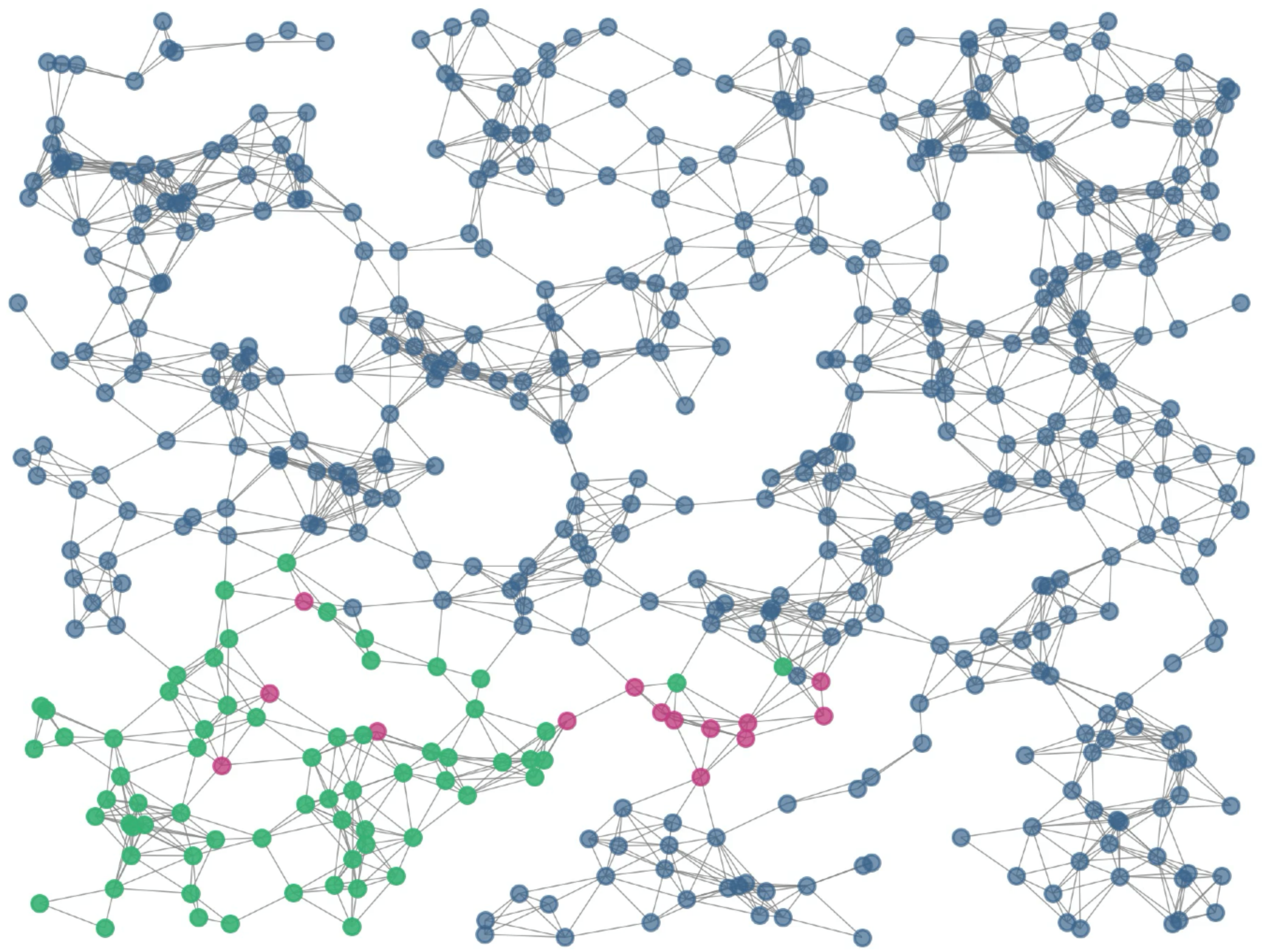

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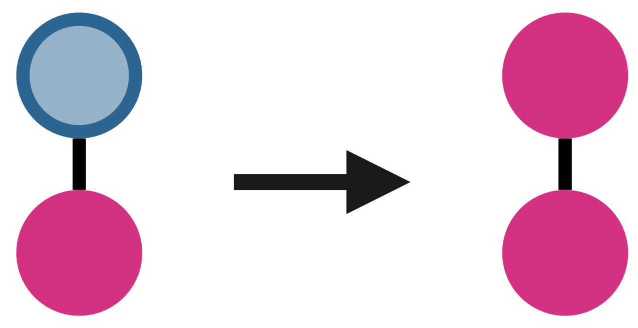

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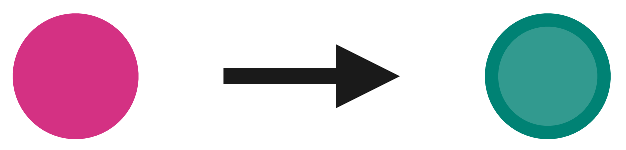

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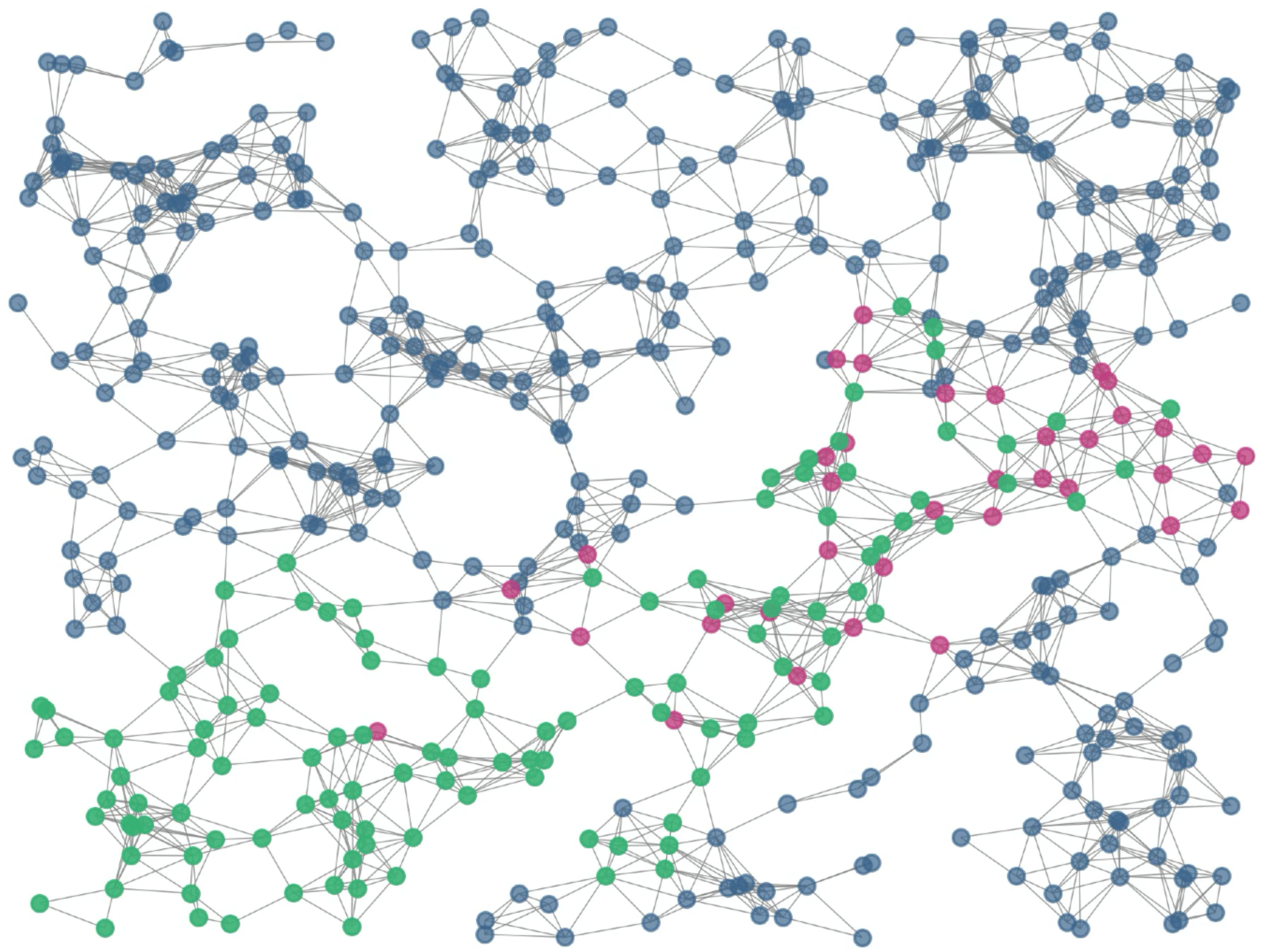

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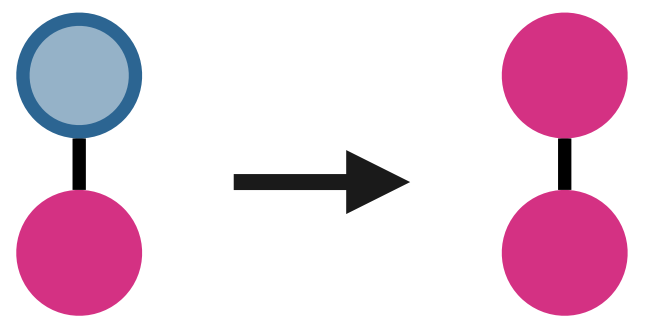

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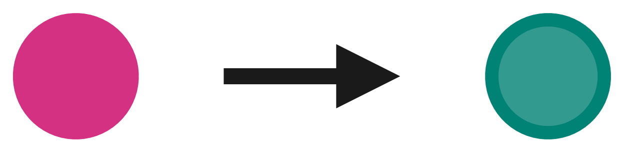

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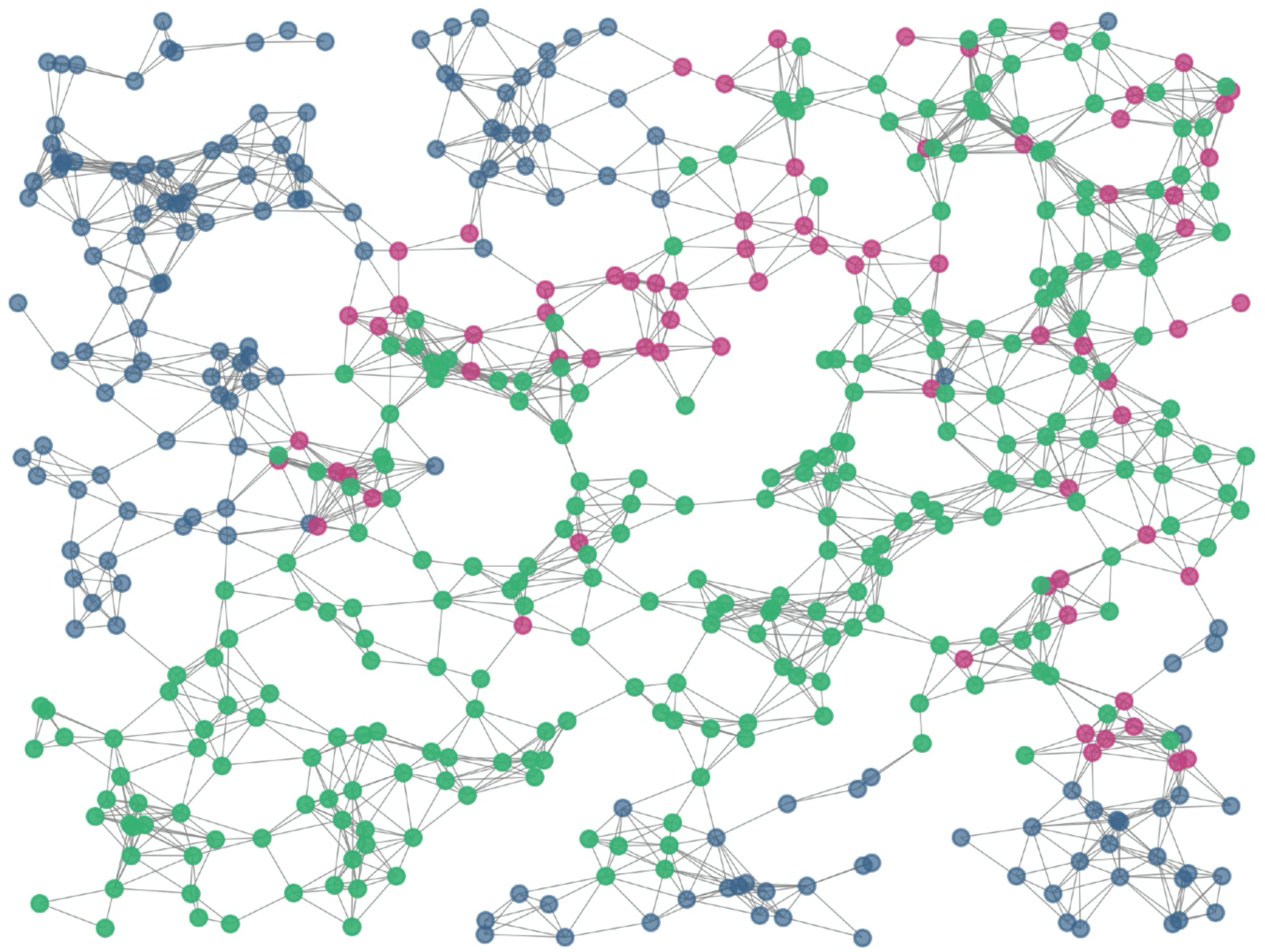

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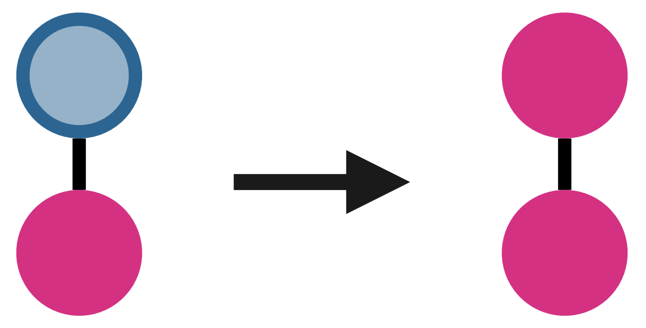

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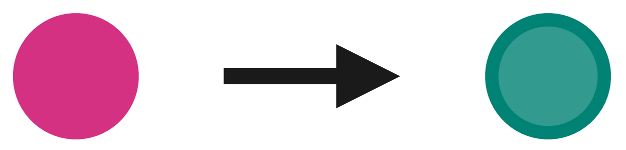

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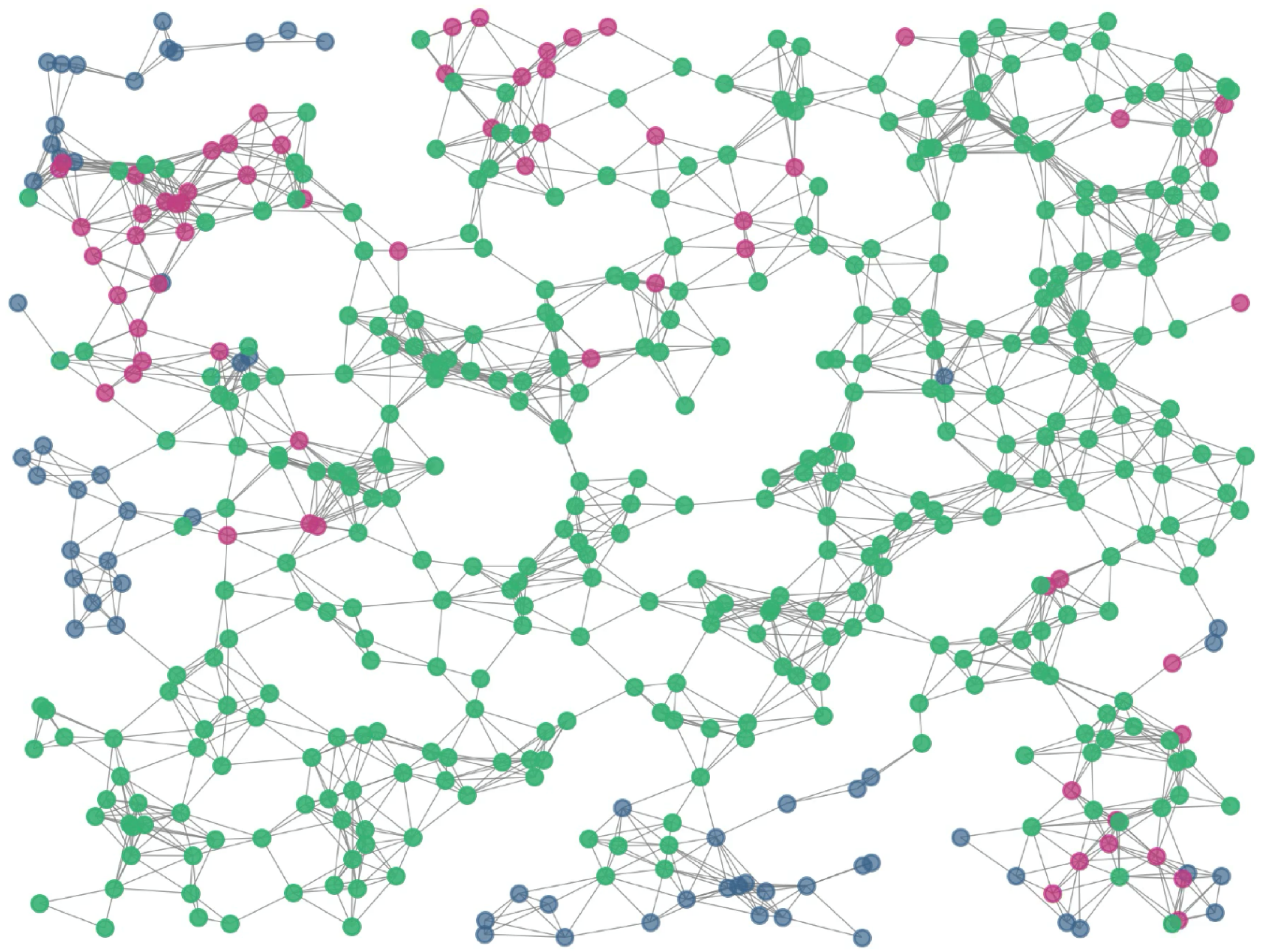

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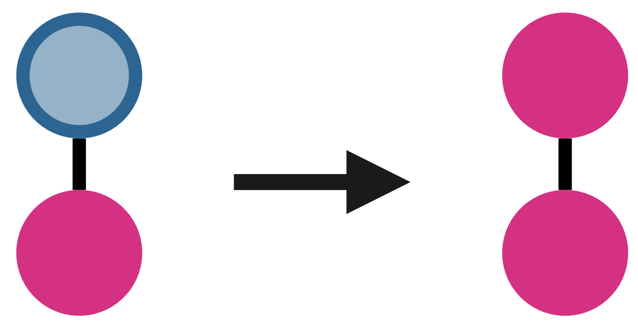

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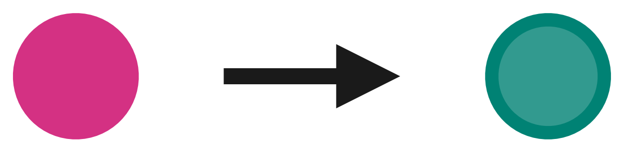

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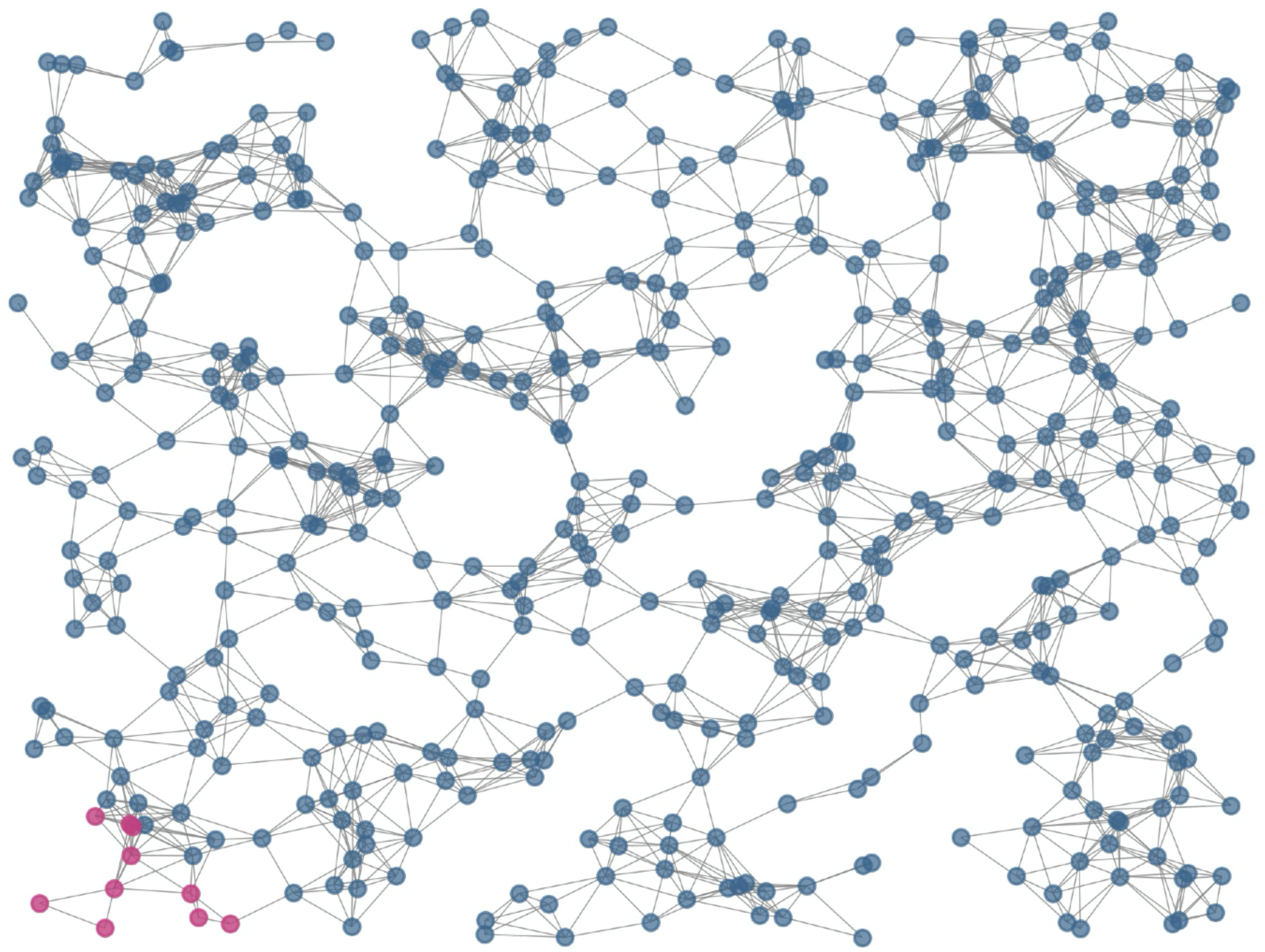
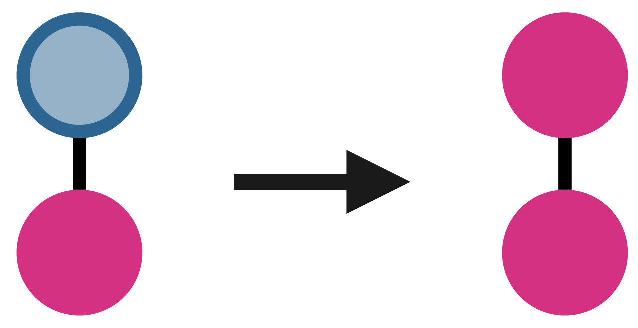
SIS



- Nodes are infected or susceptible.



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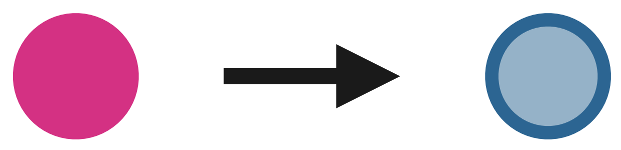

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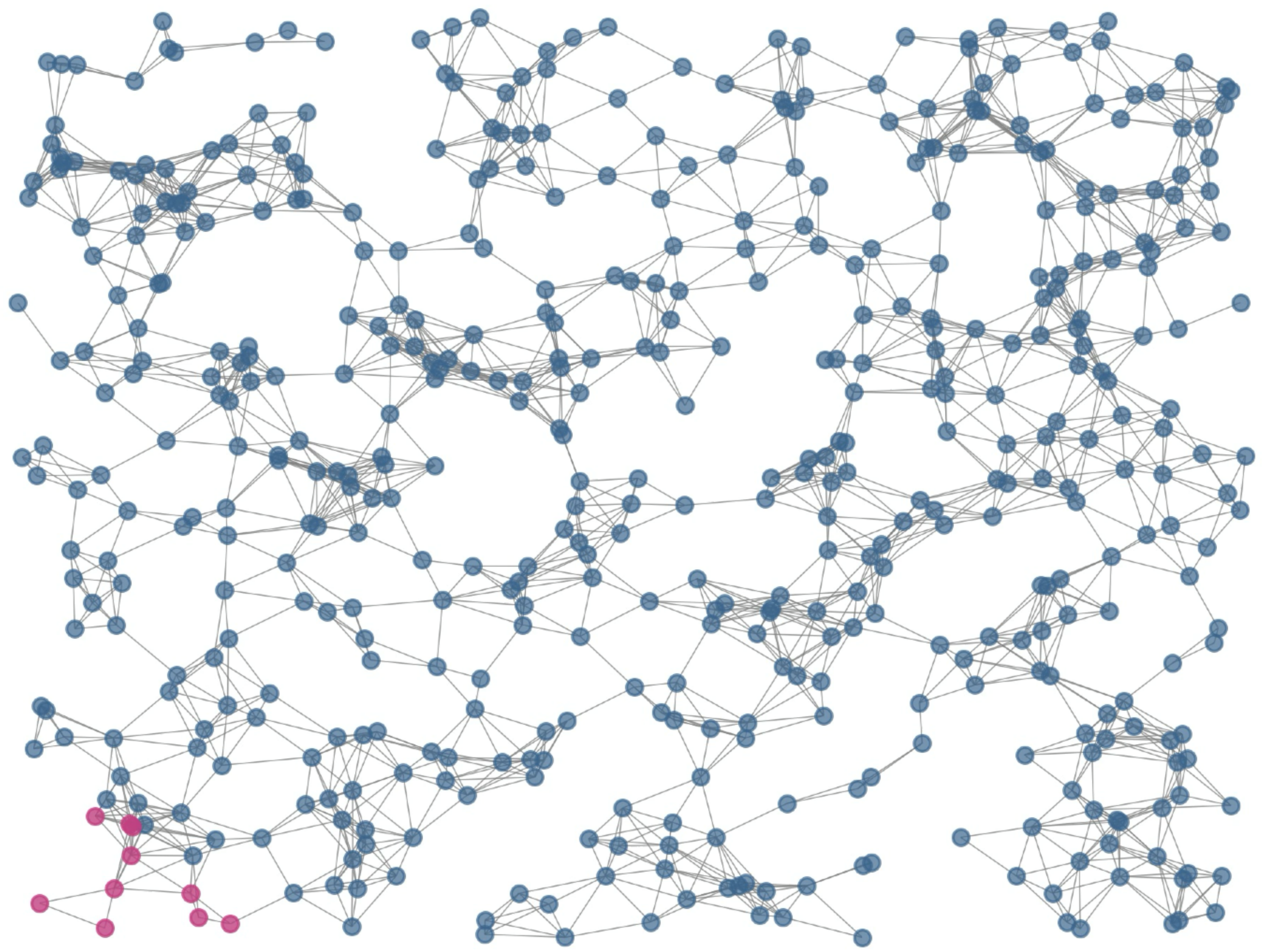

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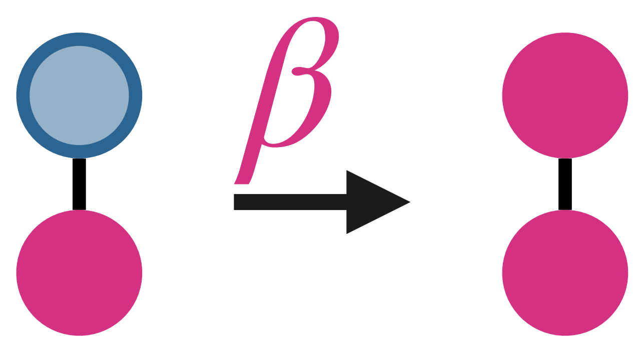

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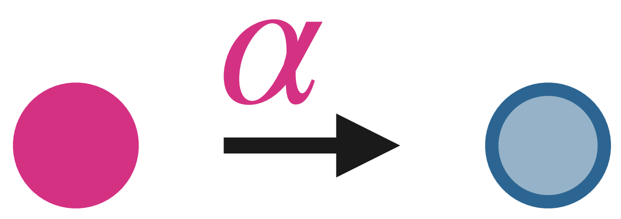

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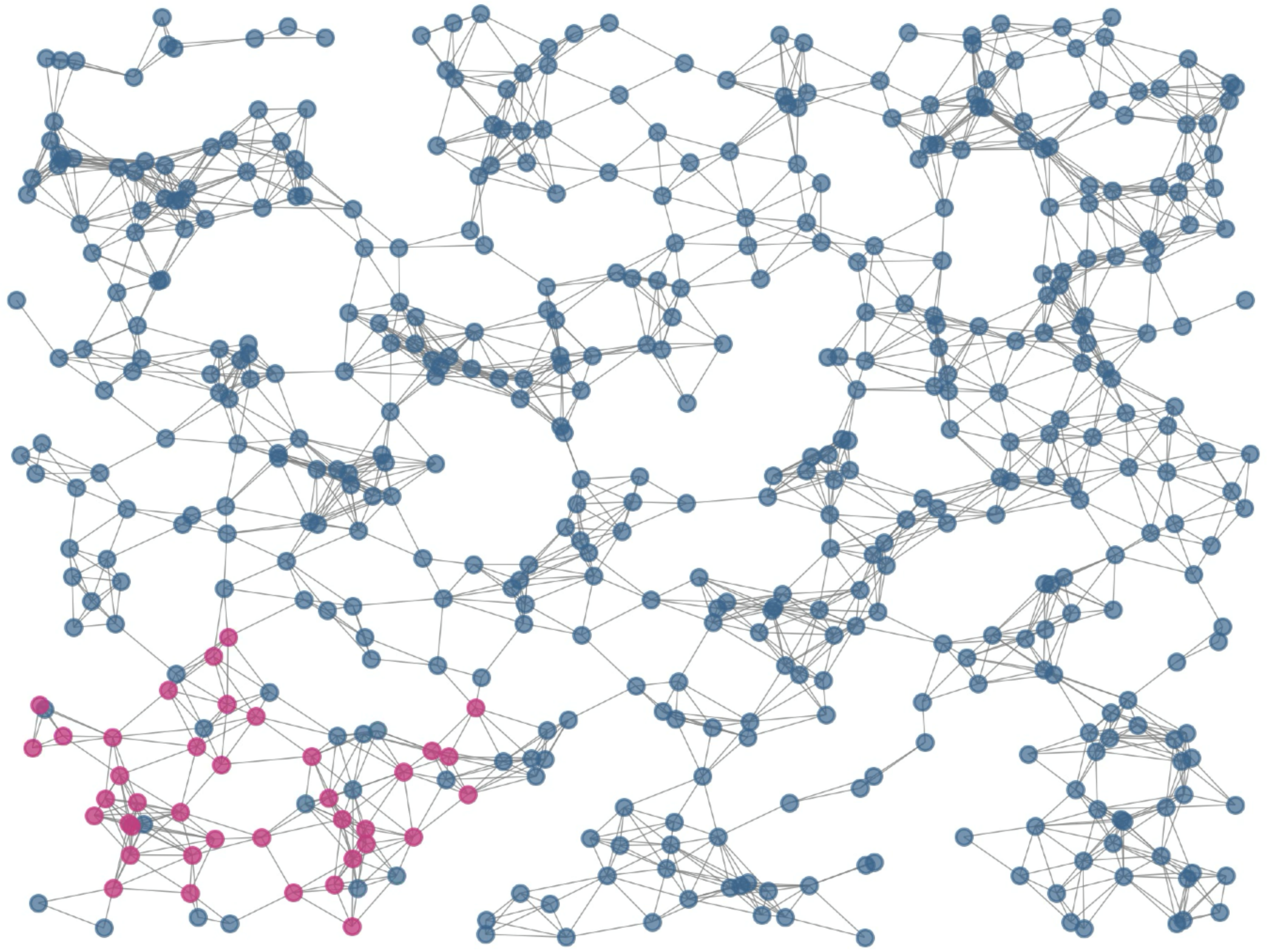
- **Continuous-time stochastic jump process**

SIS



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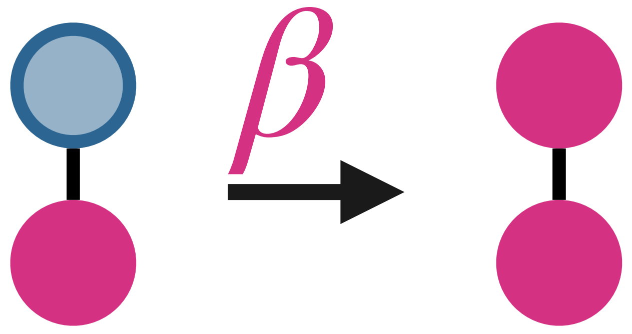

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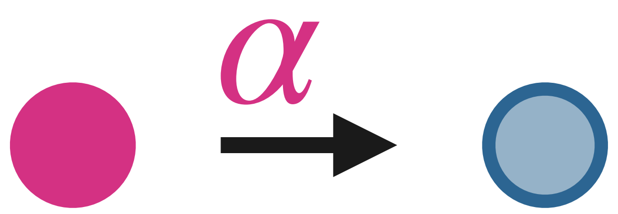

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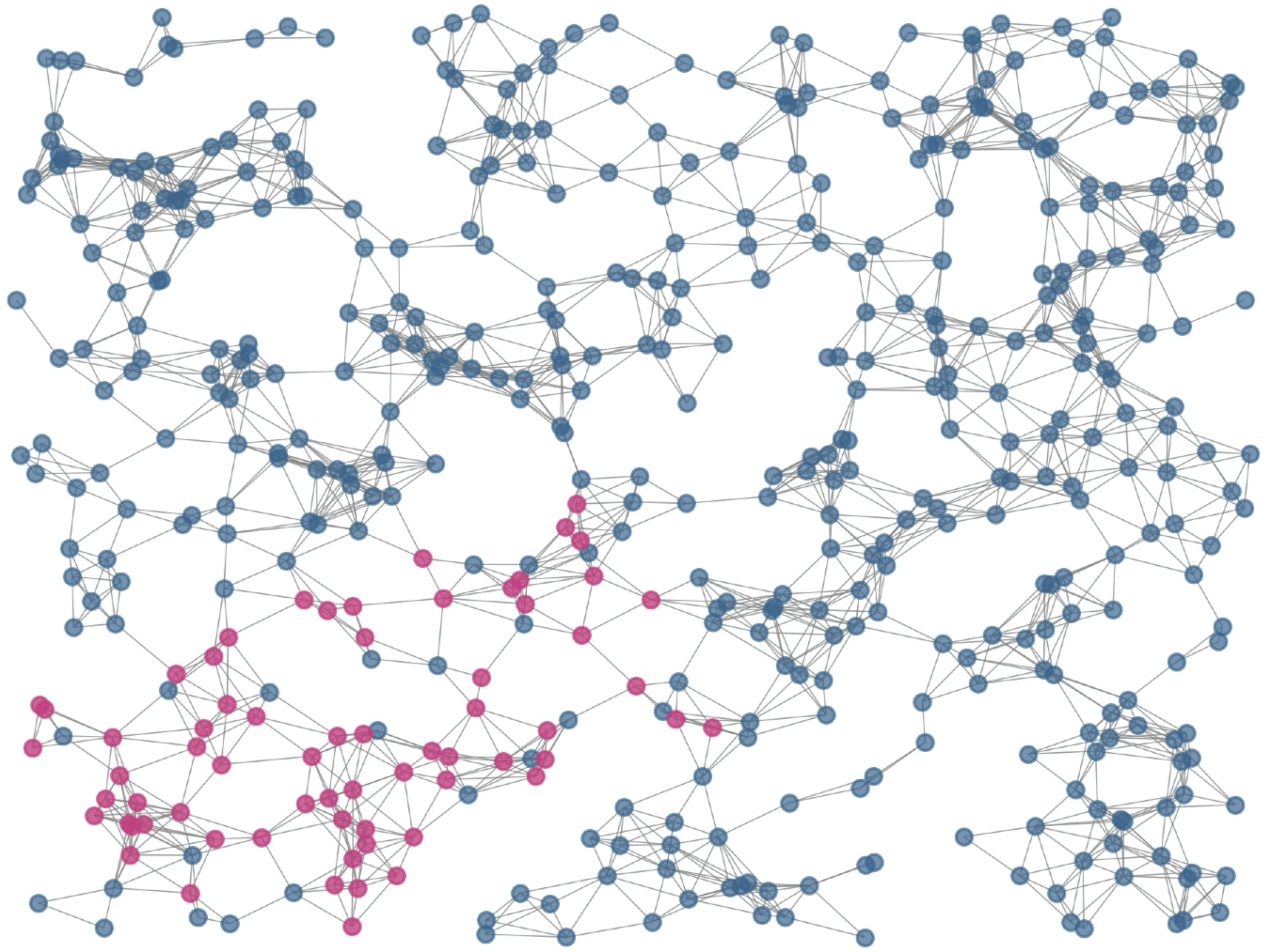

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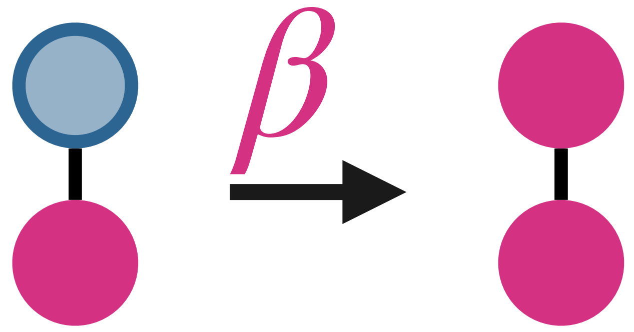

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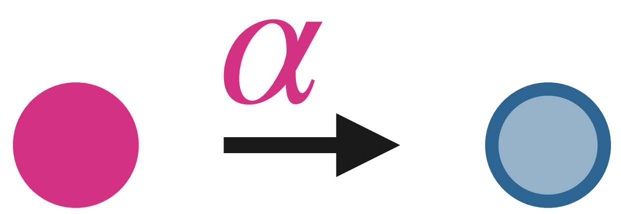

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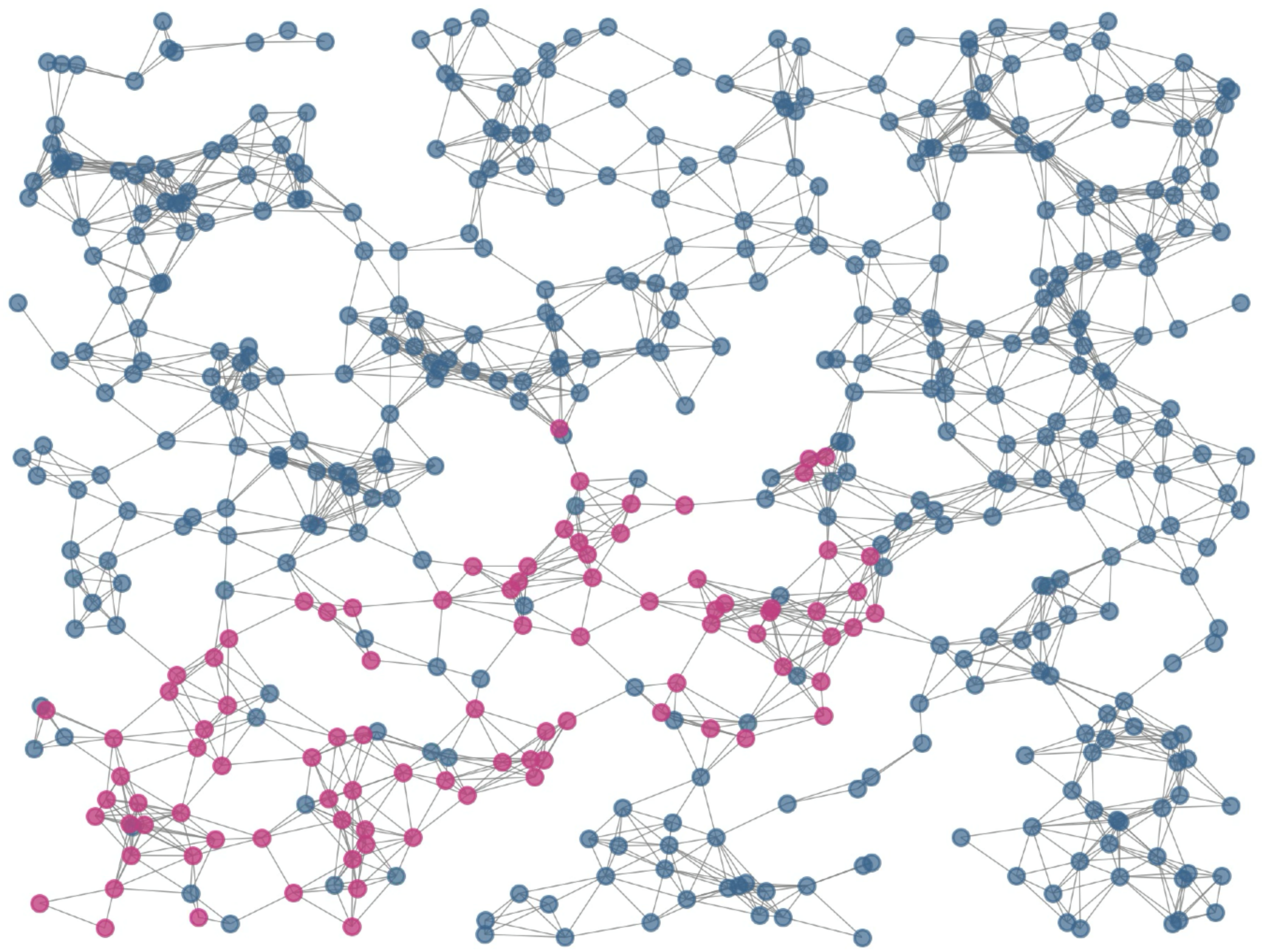

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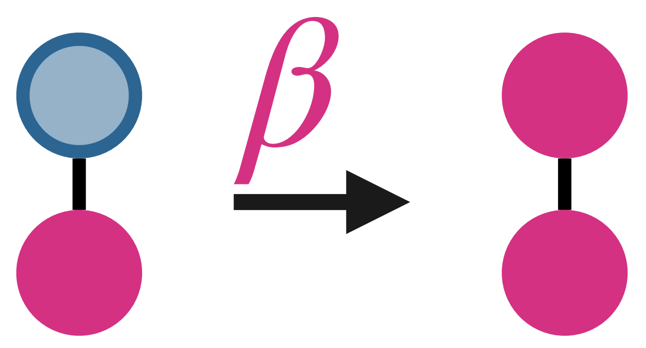

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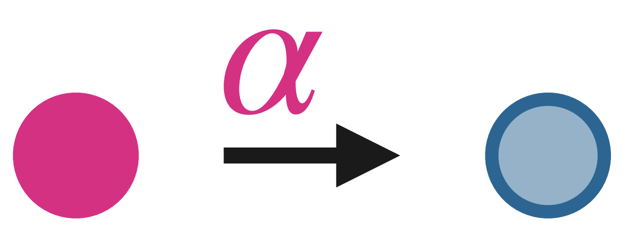

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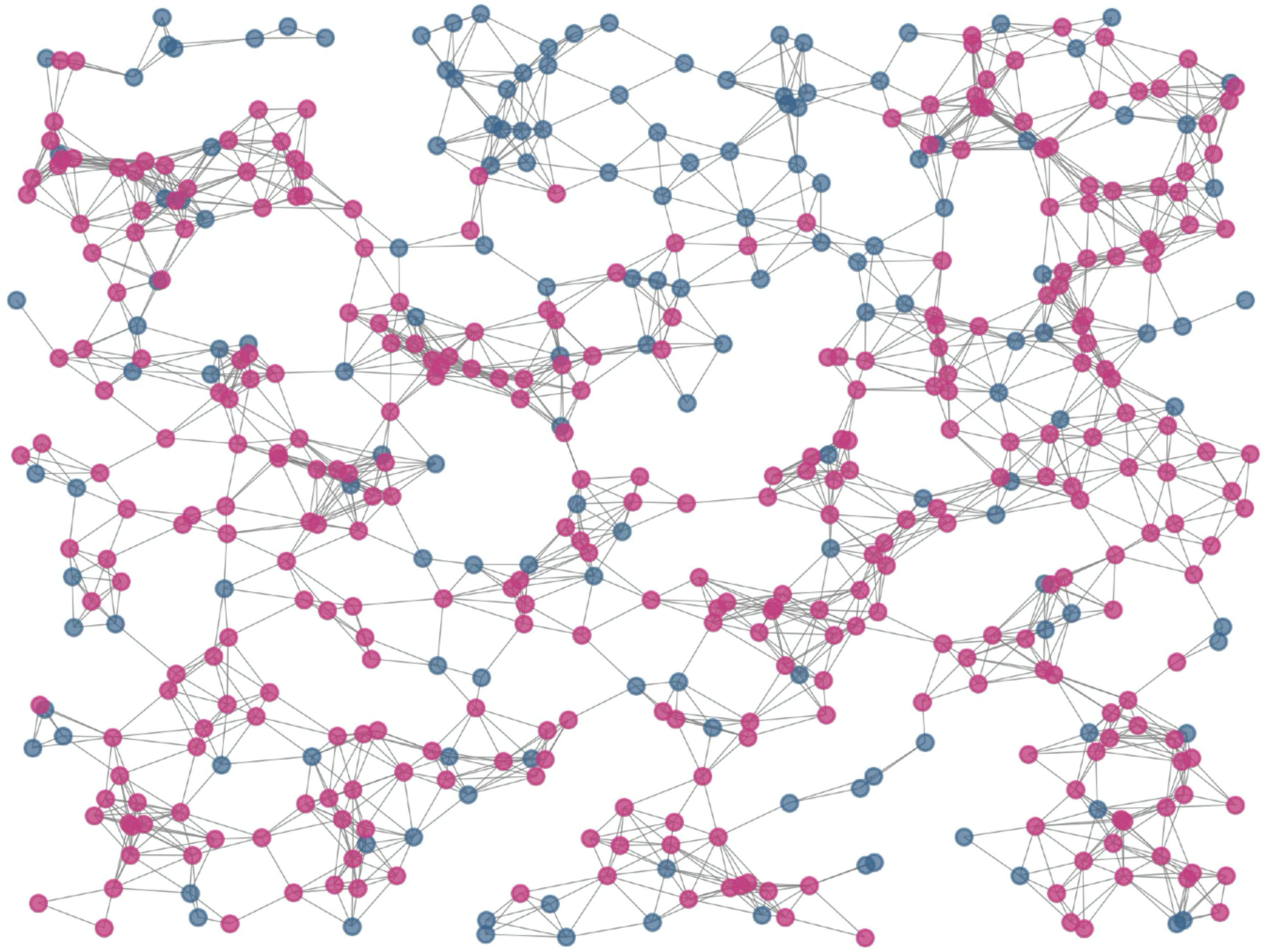

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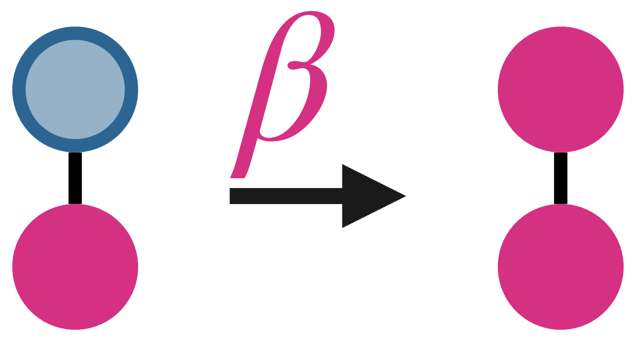

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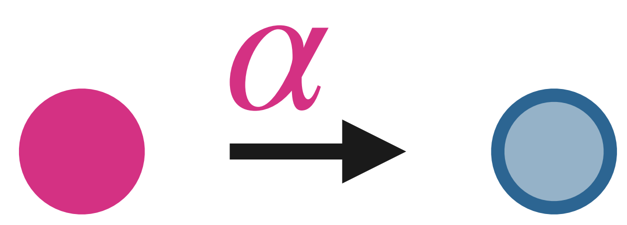

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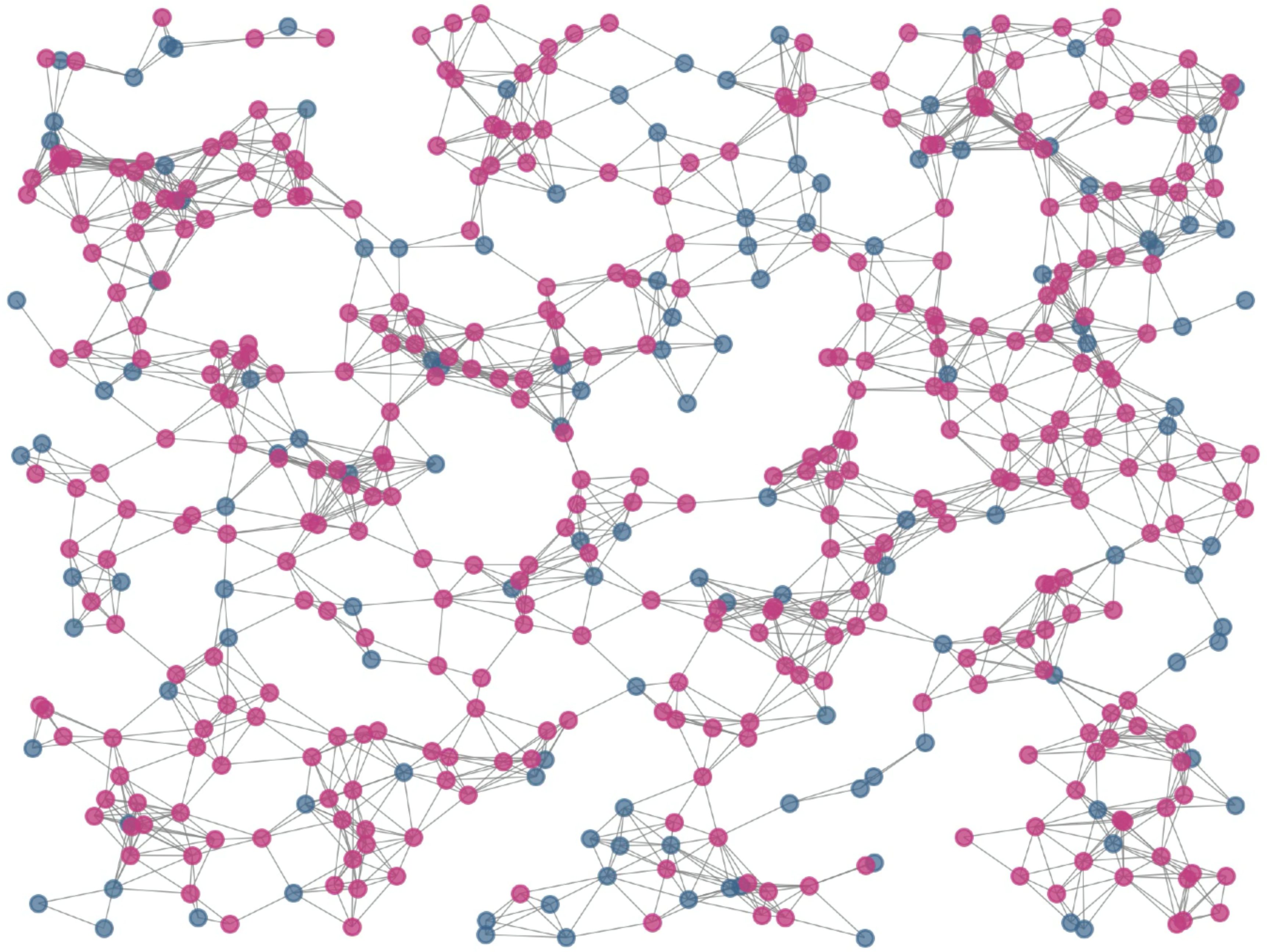

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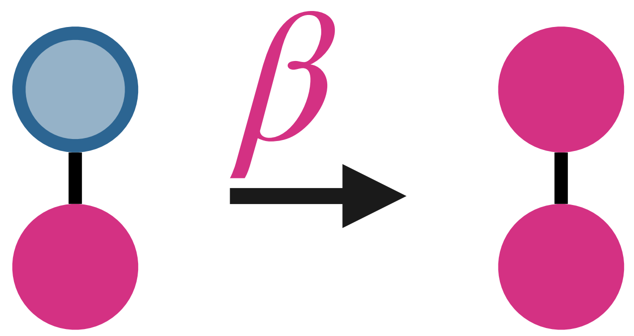

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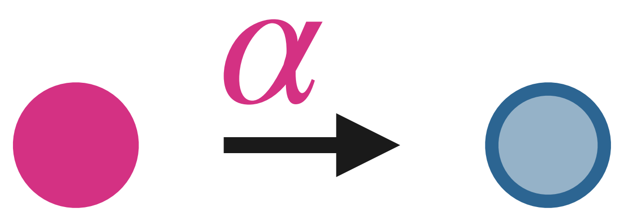

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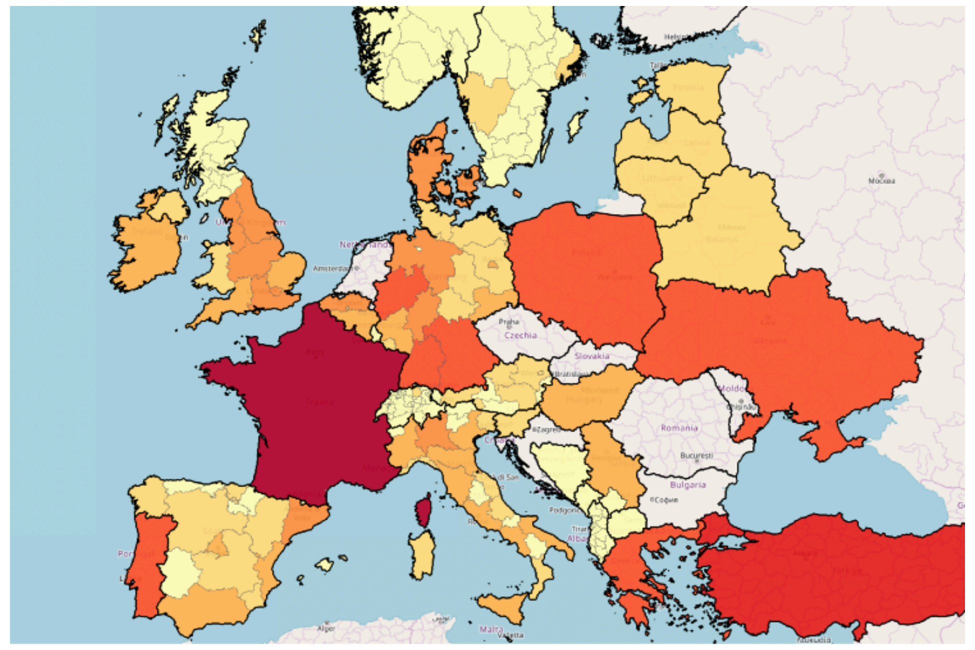
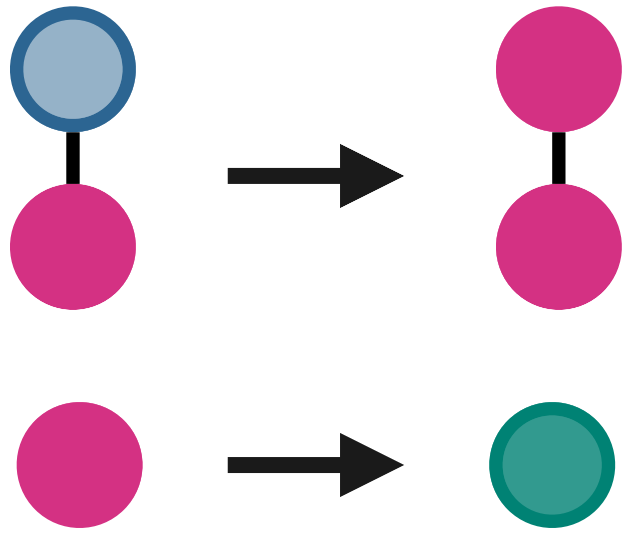
Pipeline





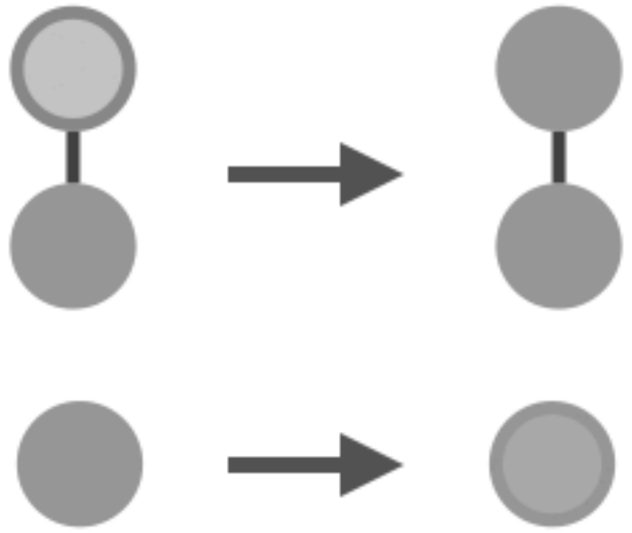
- Expected number infected individuals?
- Final epidemic size?
- Worst case number of casualties?
- Reduce the number of infections?

Observations **Model** **Questions**

Pipeline

Inference

Probing



- Expected number infected individuals?
- Final epidemic size?
- Worst case number of casualties?
- Reduce the number of infections?

Observations

Model

Questions

Agenda

METHODS

COVID

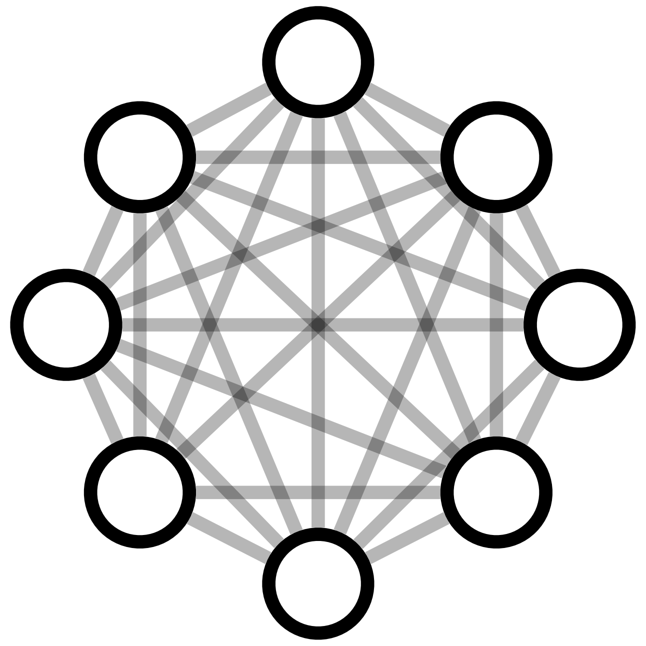
(NON-)MARKOVIAN SIMULATION

CONTROL

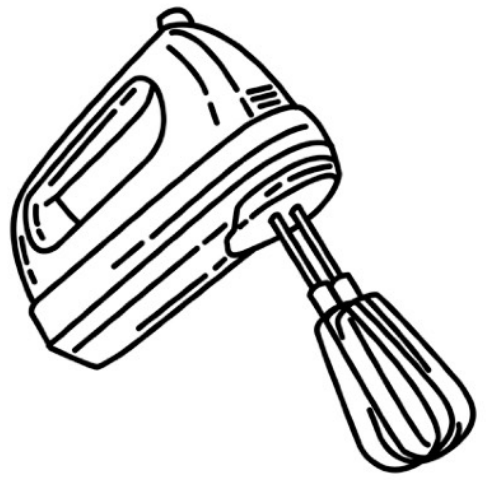
INFERENCE

Networks - Why Do We Care?

Homogenous connectivity:



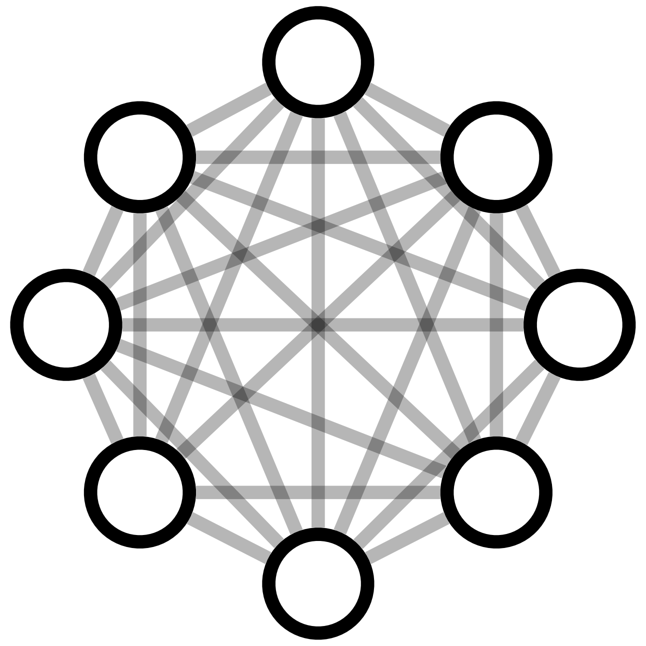
Every one is connected with everyone else “a little bit”.



Well-stirred analogy

Networks - Why Do We Care?

Homogenous connectivity:



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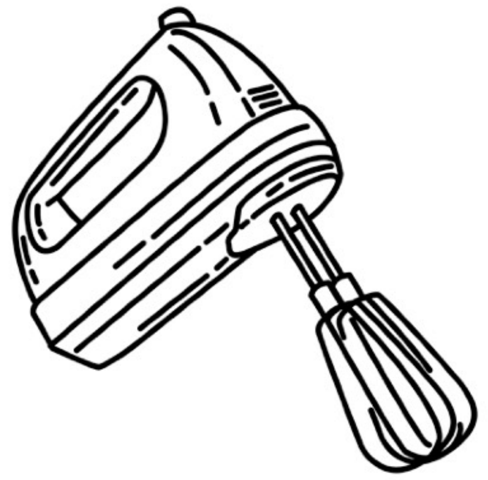
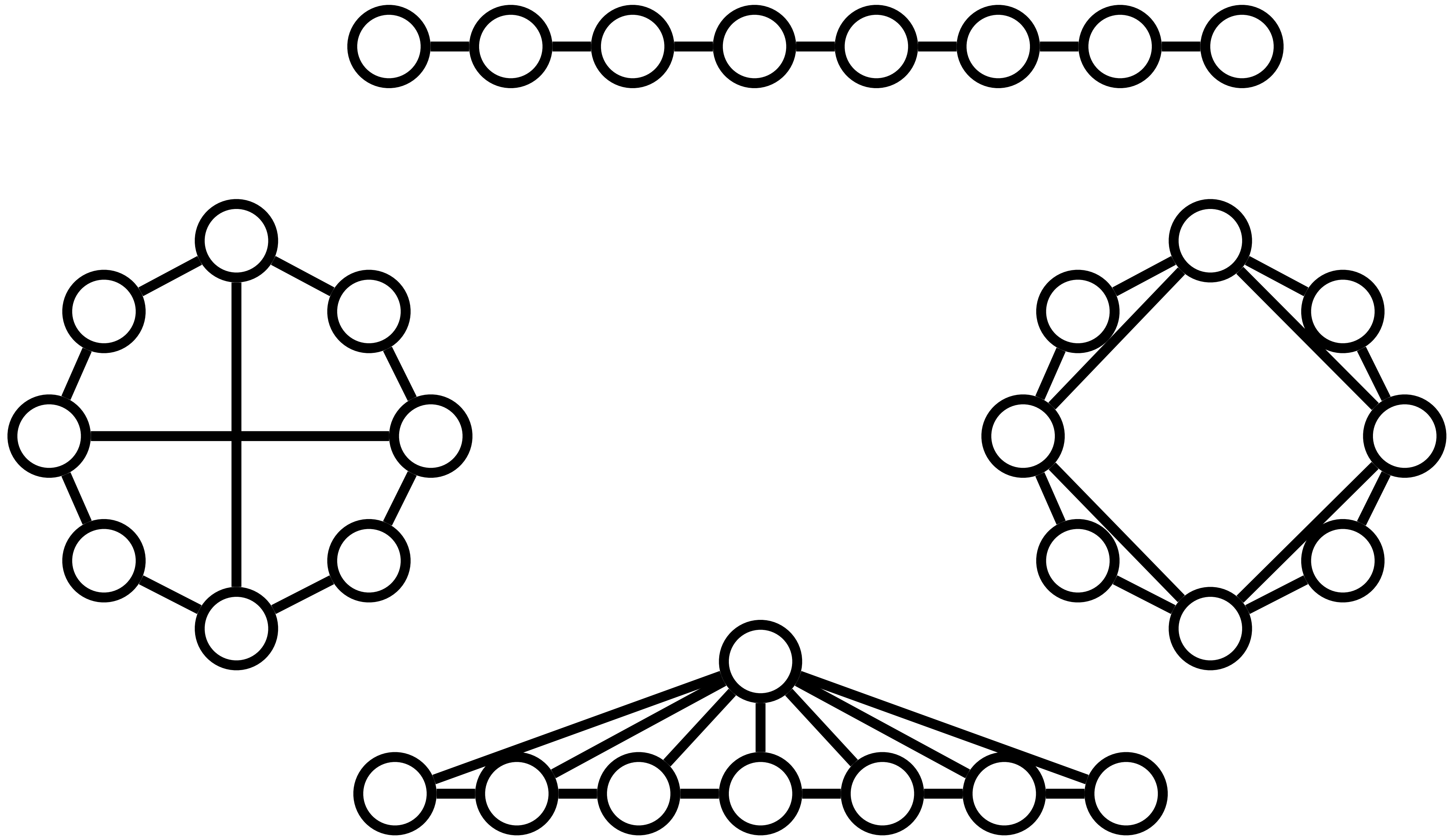


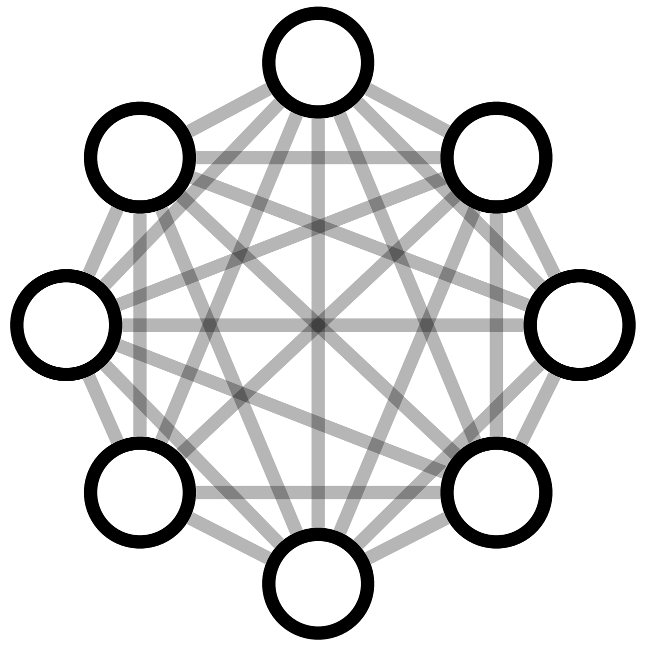
Well-stirred analogy

Network-constrained connectivity:



Networks - Why Do We Care?

Homogenous connectivity:



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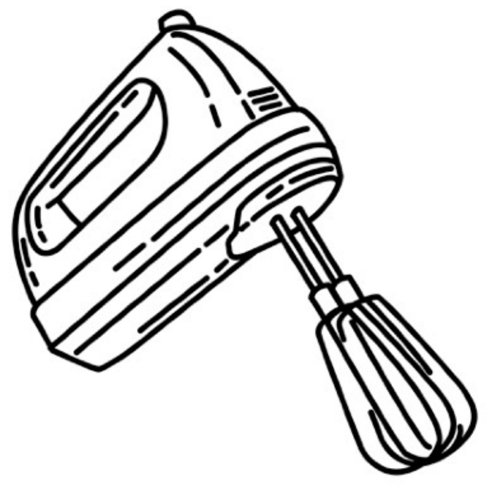
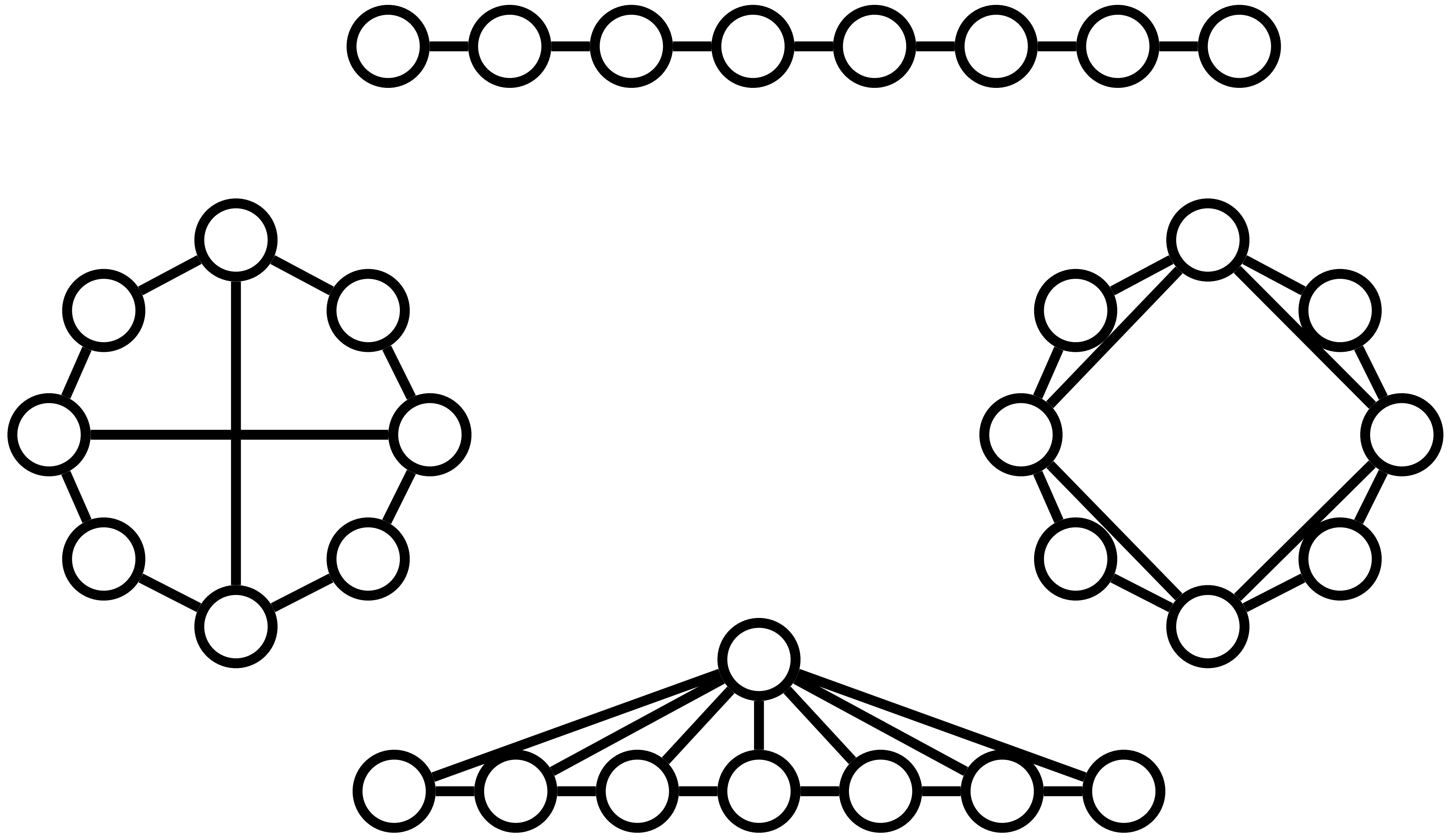


Well-stirred analogy

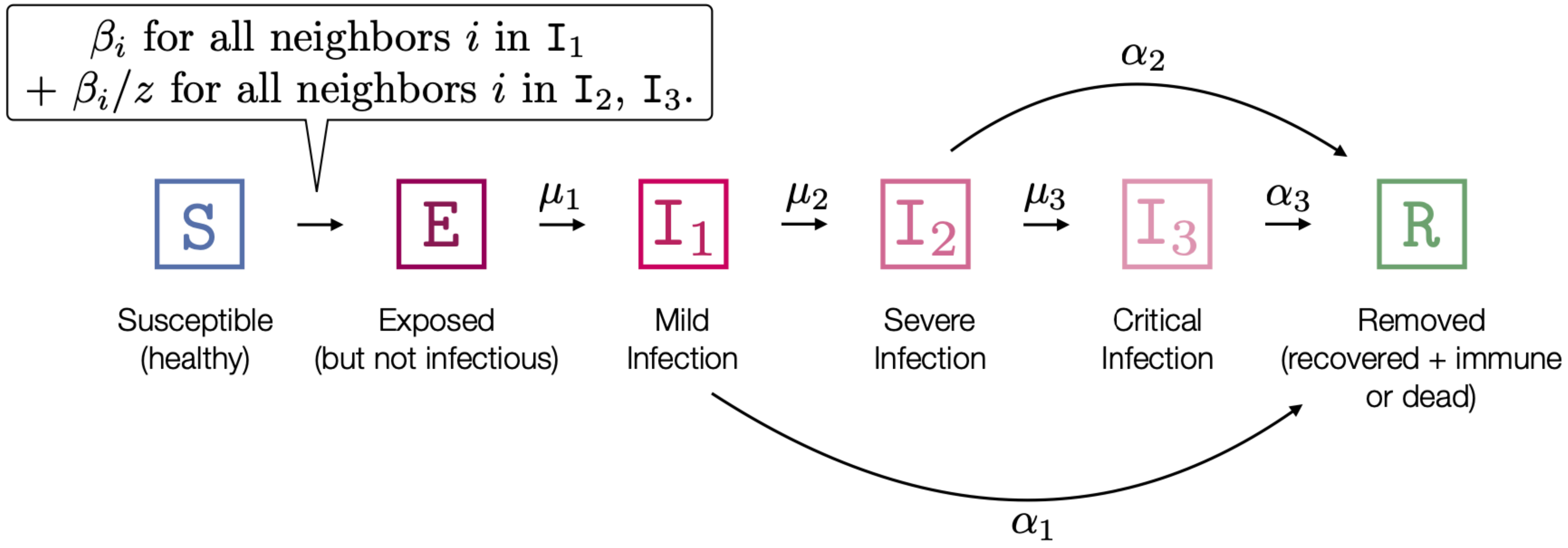
Network-constrained connectivity:



Spreading on network is very different from spreading in a homogenous population.

Covid-19

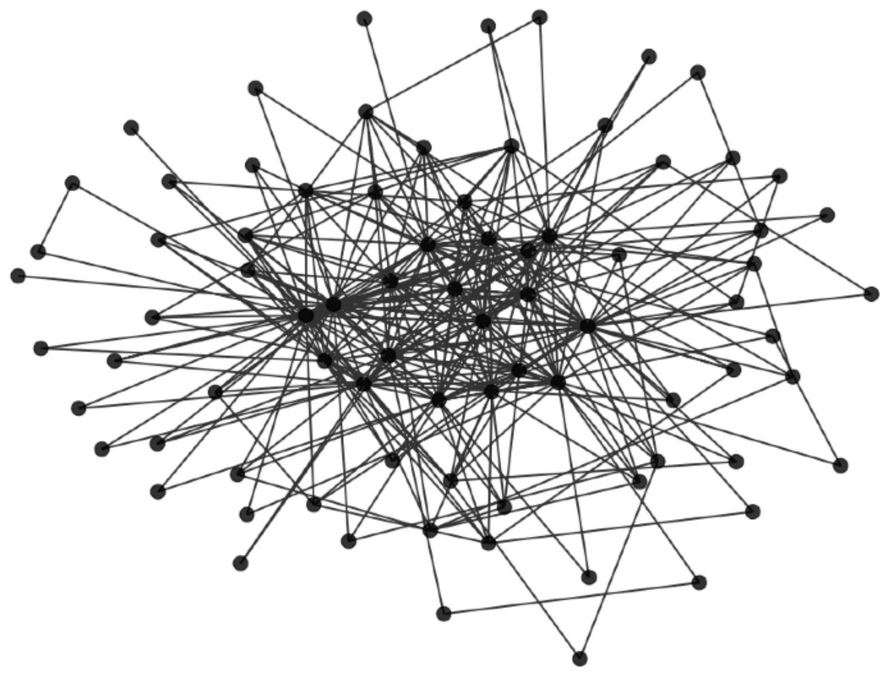
Adopt **SIR** model for Covid-19:



Nande et al. (2021)

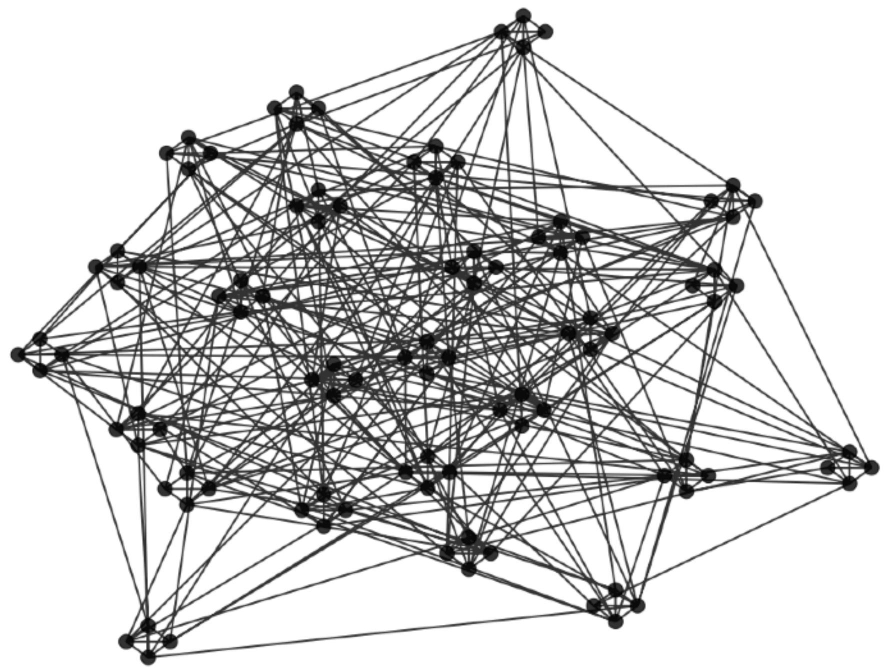
Covid-19

Test different networks types (fixed mean degree):



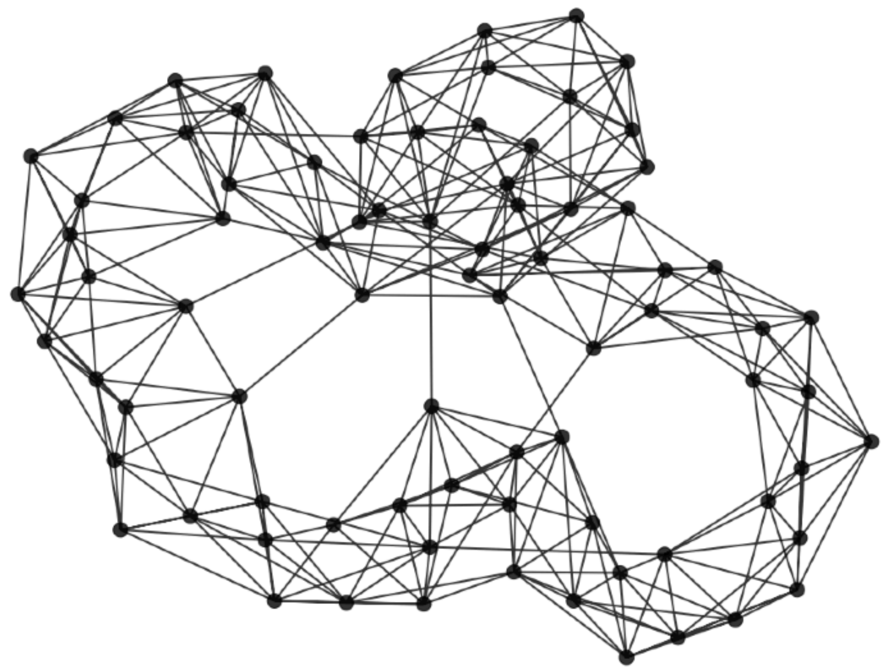
Power-law

- Small number of hubs
- Many nodes with very few neighbors



Household

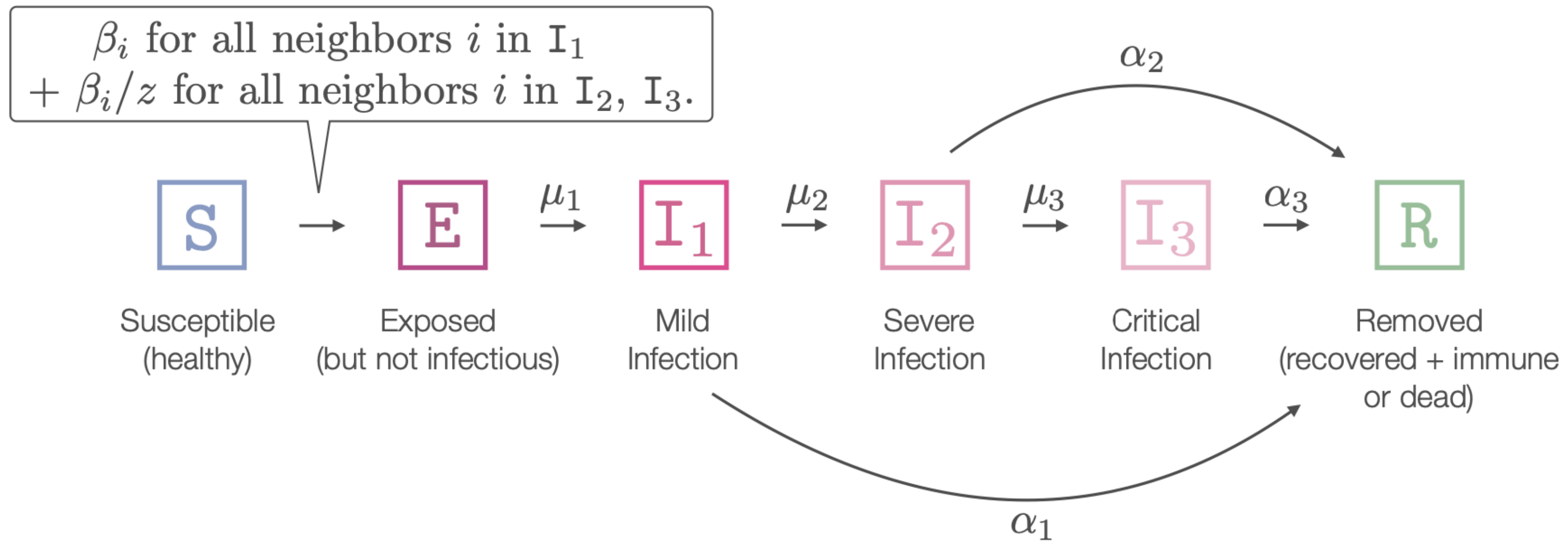
- Household size = 4
- Connected via a Geometric network



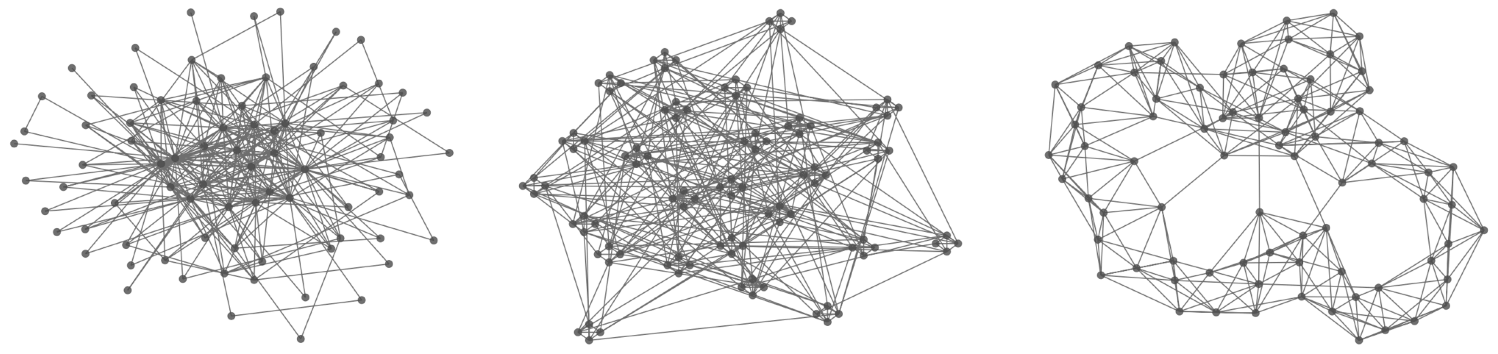
Watts-Strogatz

- Fixed number of contacts
- Small-world

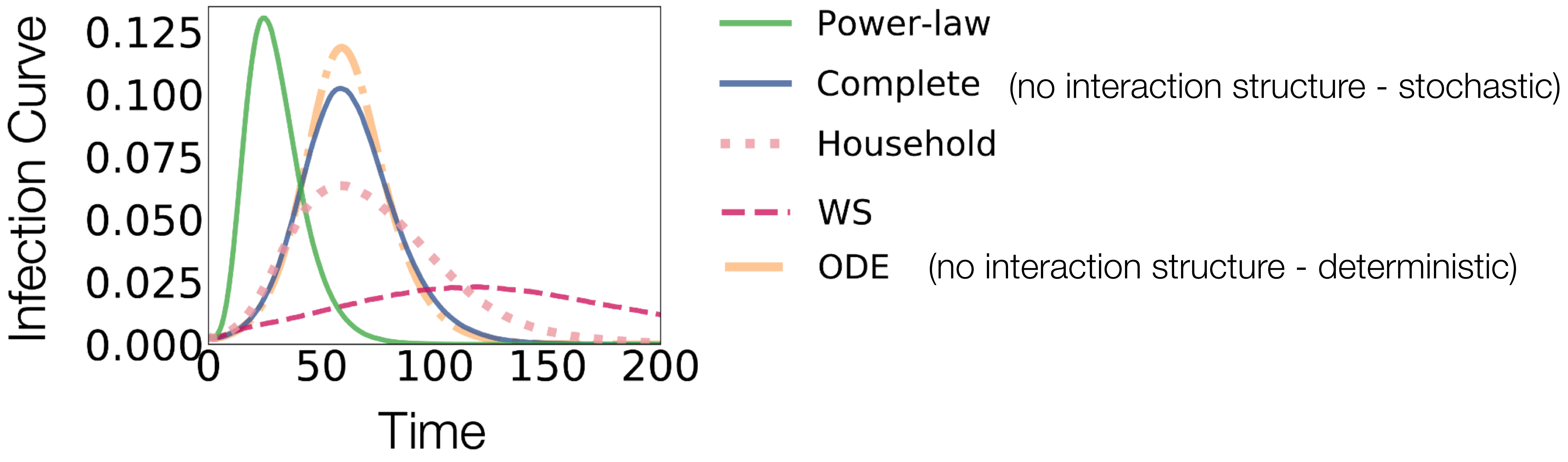
Covid-19



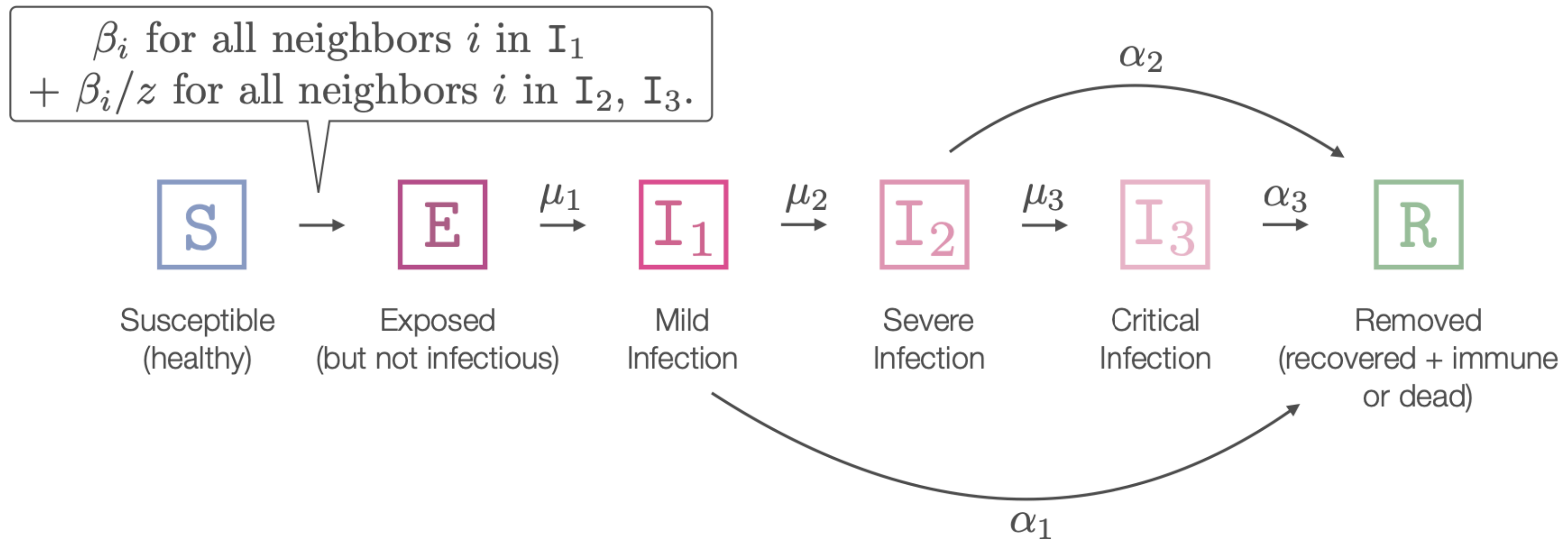
Fix basic reproduction number R_0.



Power-law | Household | Watts-Strogatz



Covid-19



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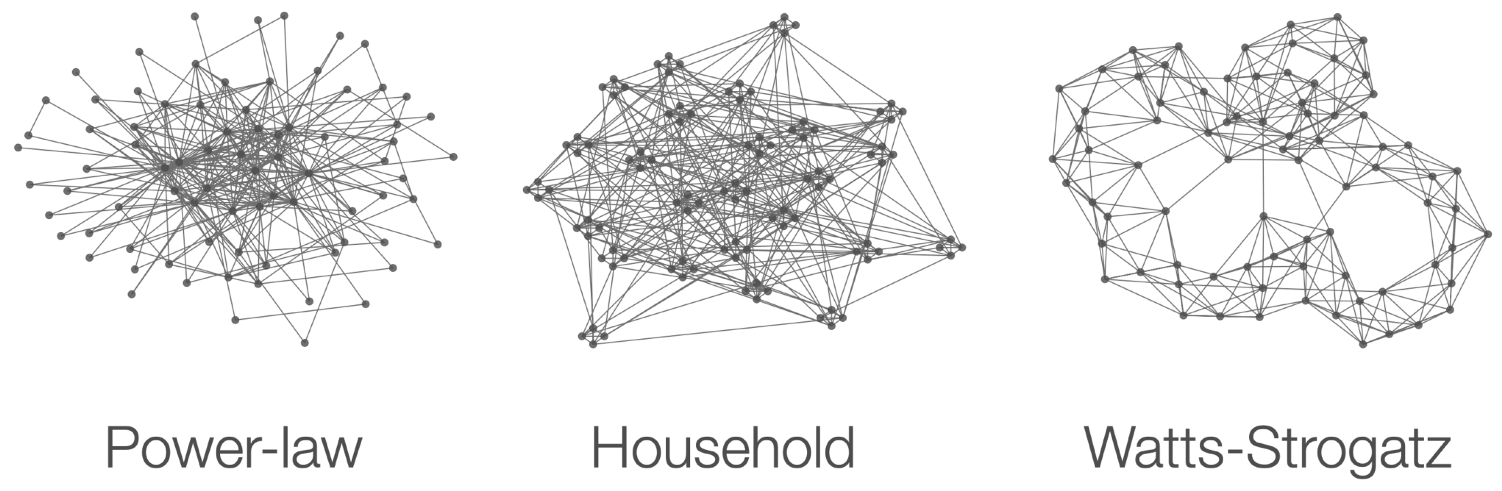
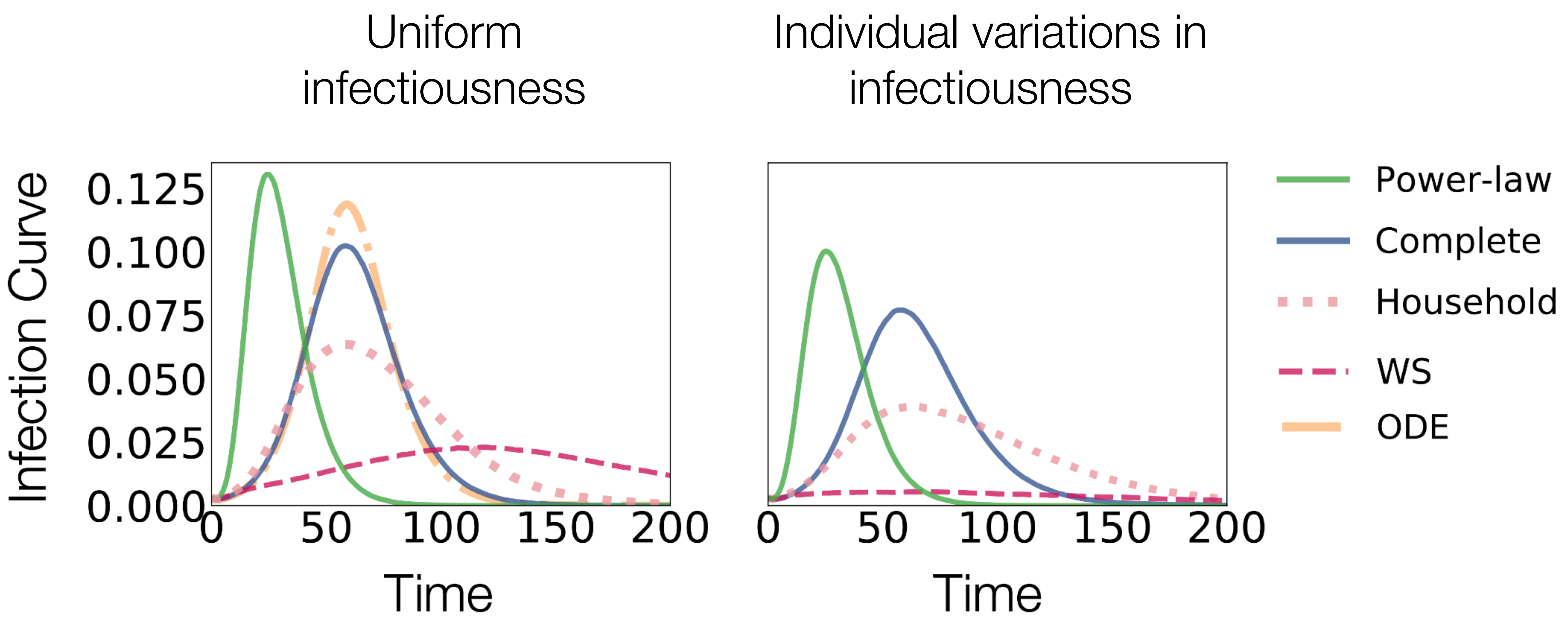
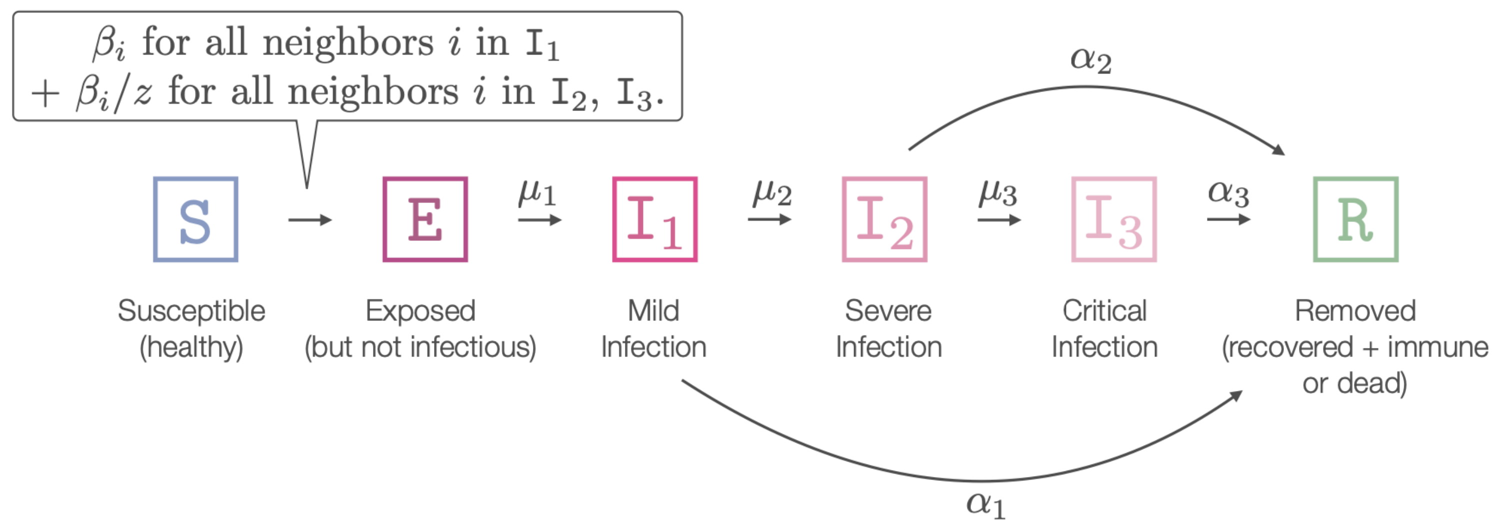
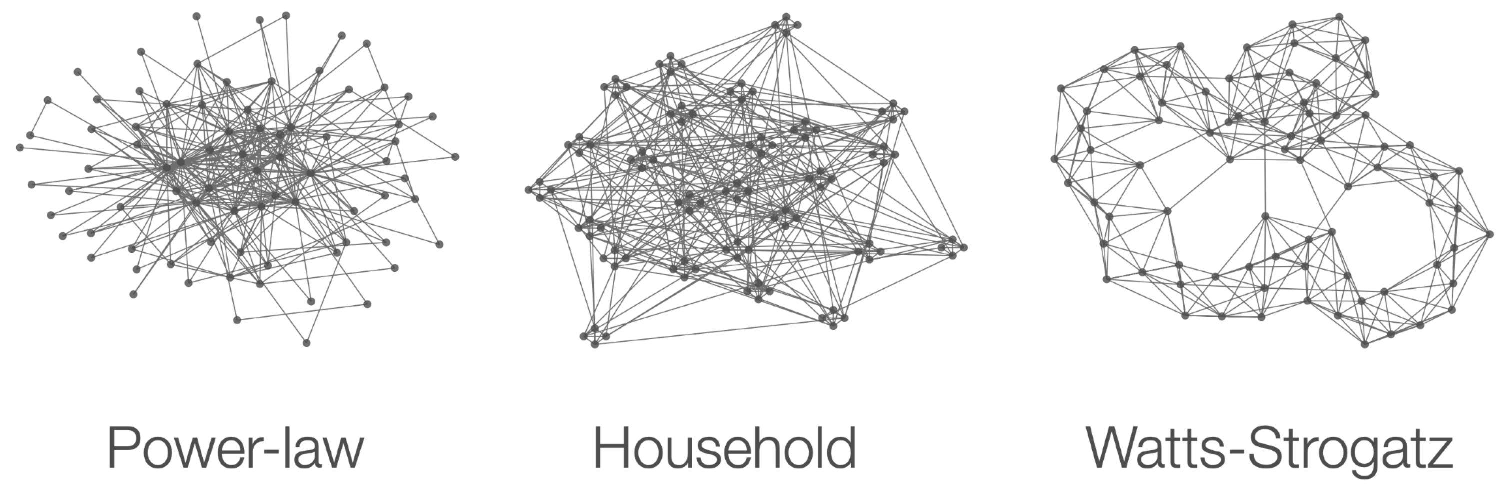
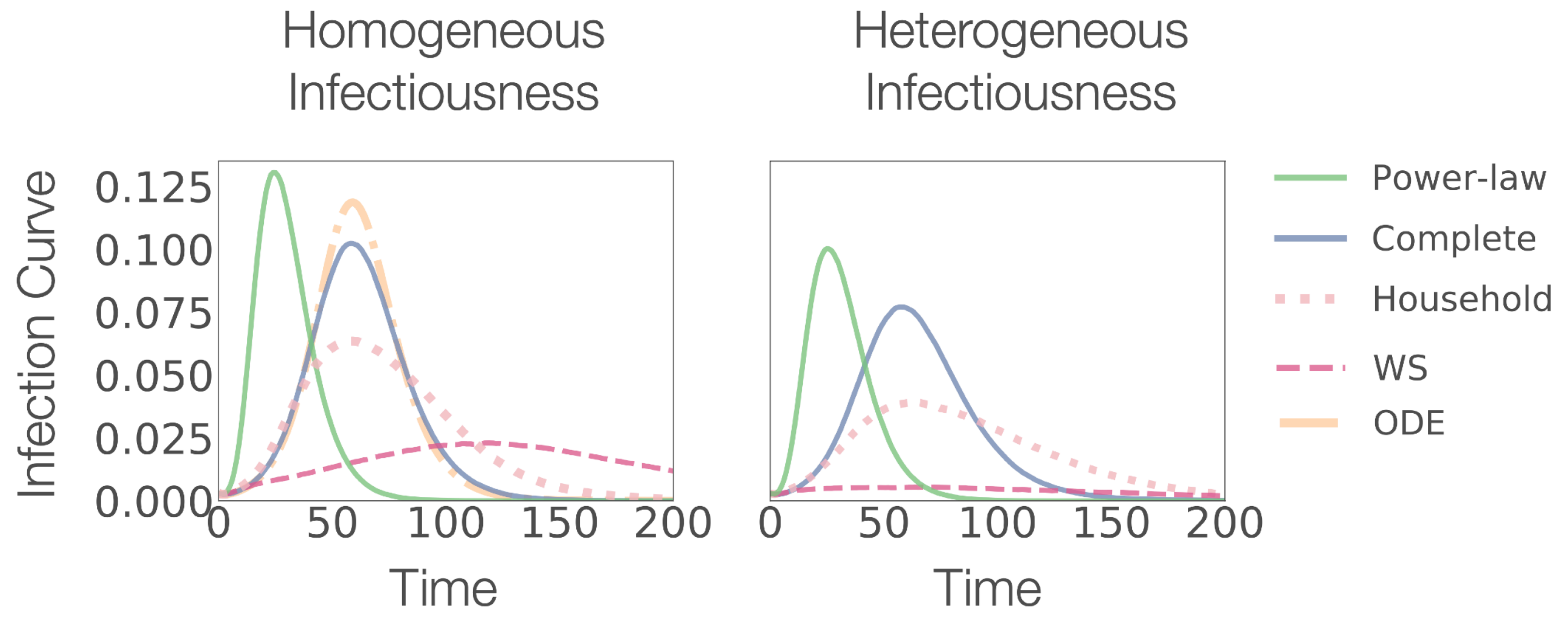




Covid-19







- **Do not use population averages** to describe a population (mean number of contacts, mean infectiousness).
- **Vast differences** in all relevant properties among networks (infection curve, Rt, dispersion, deaths)
- **Network structure** vs **individual differences** vs **environment** (complex interplay hinders analysis)

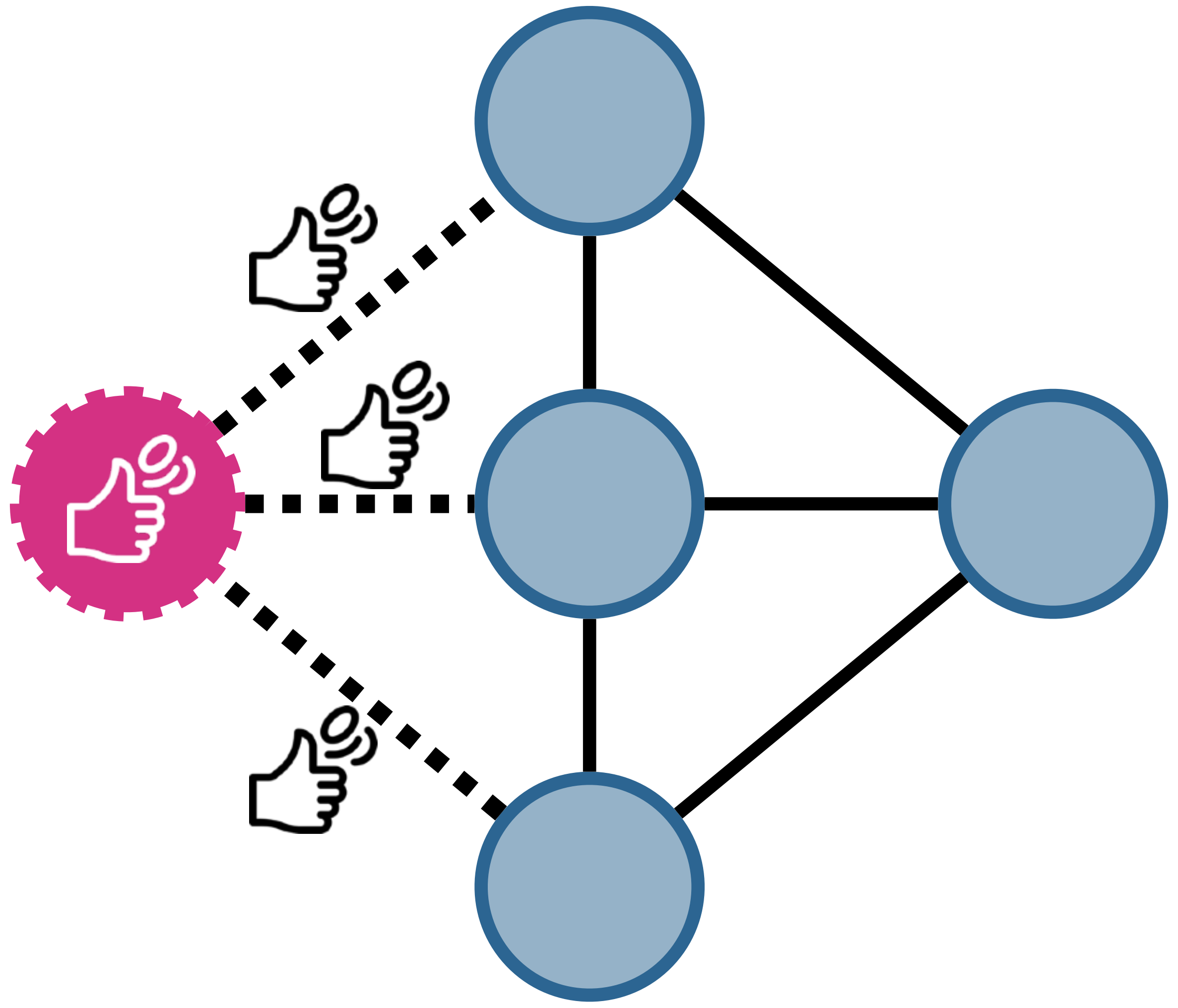
Agenda

METHODS

COVID
(NON-)MARKOVIAN SIMULATION
CONTROL
INFERENCE

SIS Simulation

naïve:



SIS Simulation

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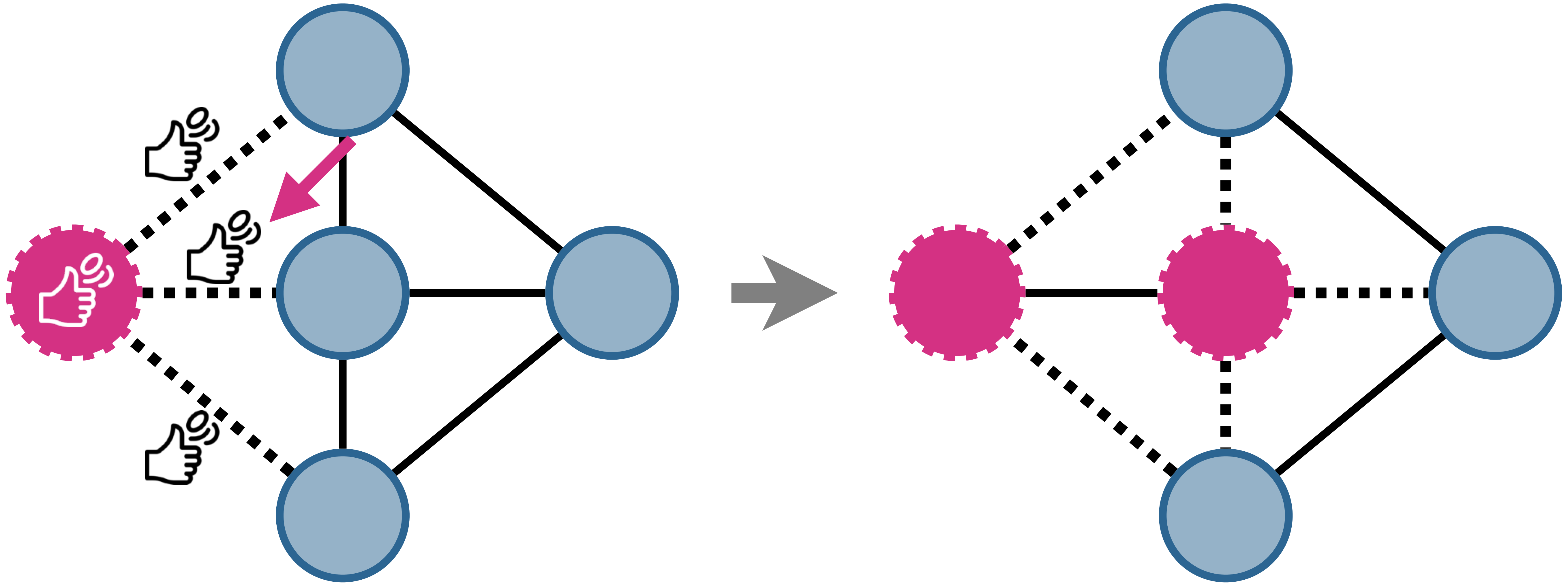

SIS Simulation

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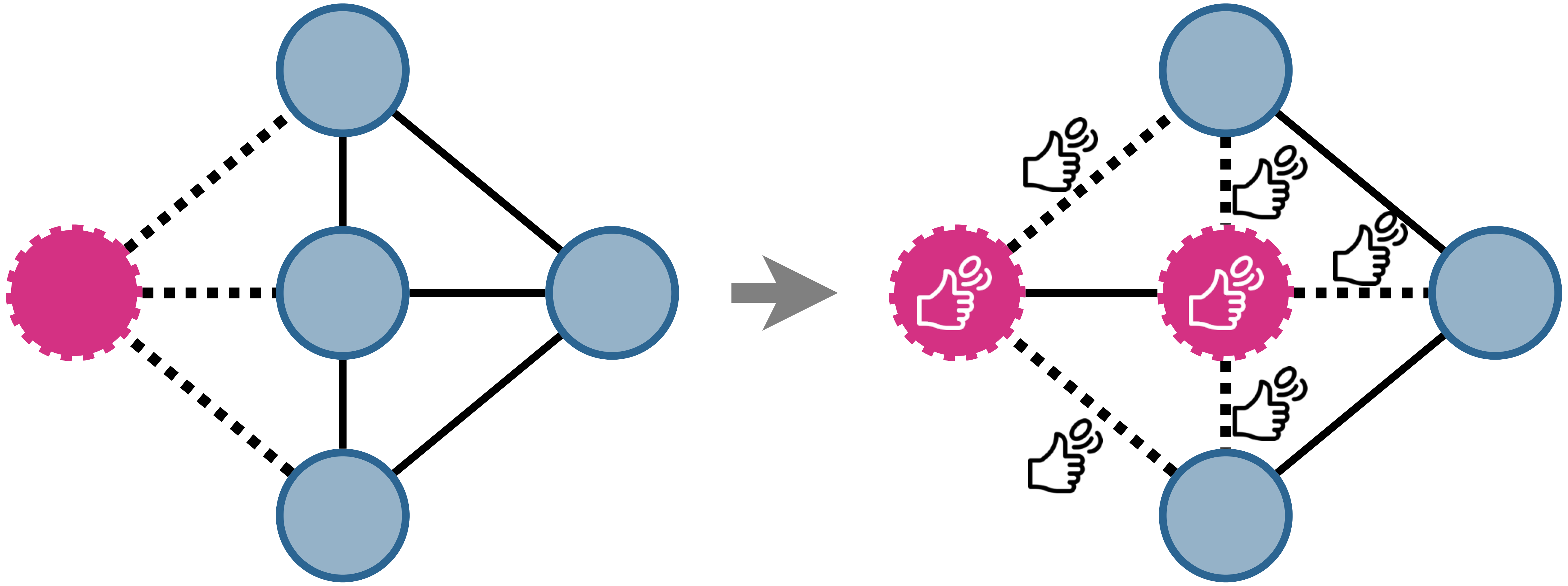

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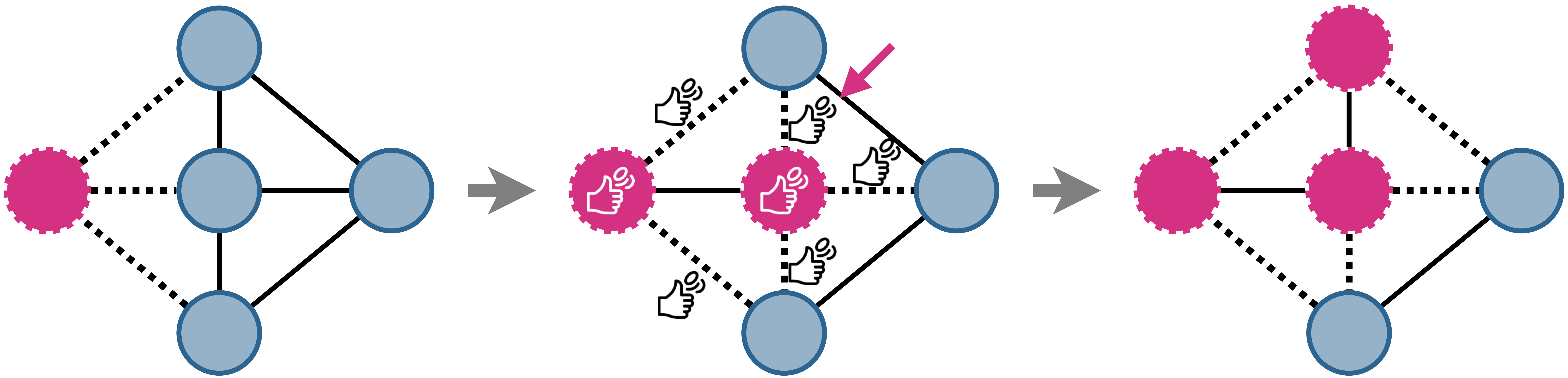

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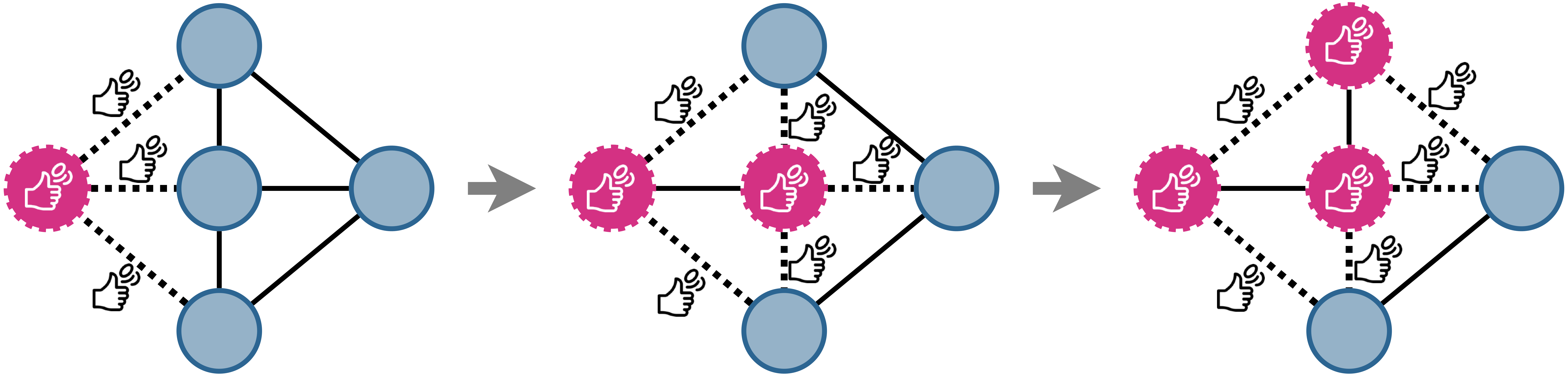
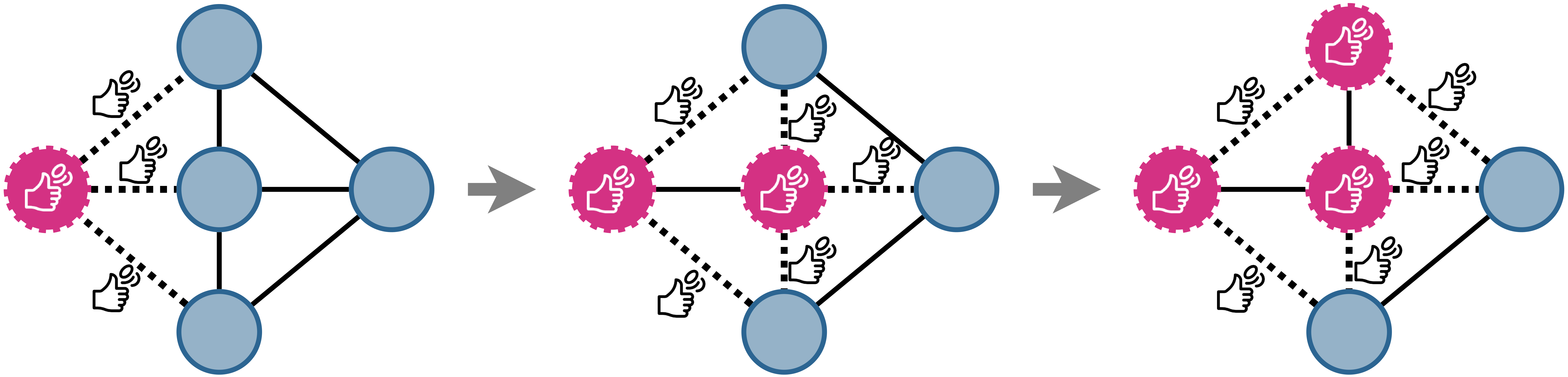


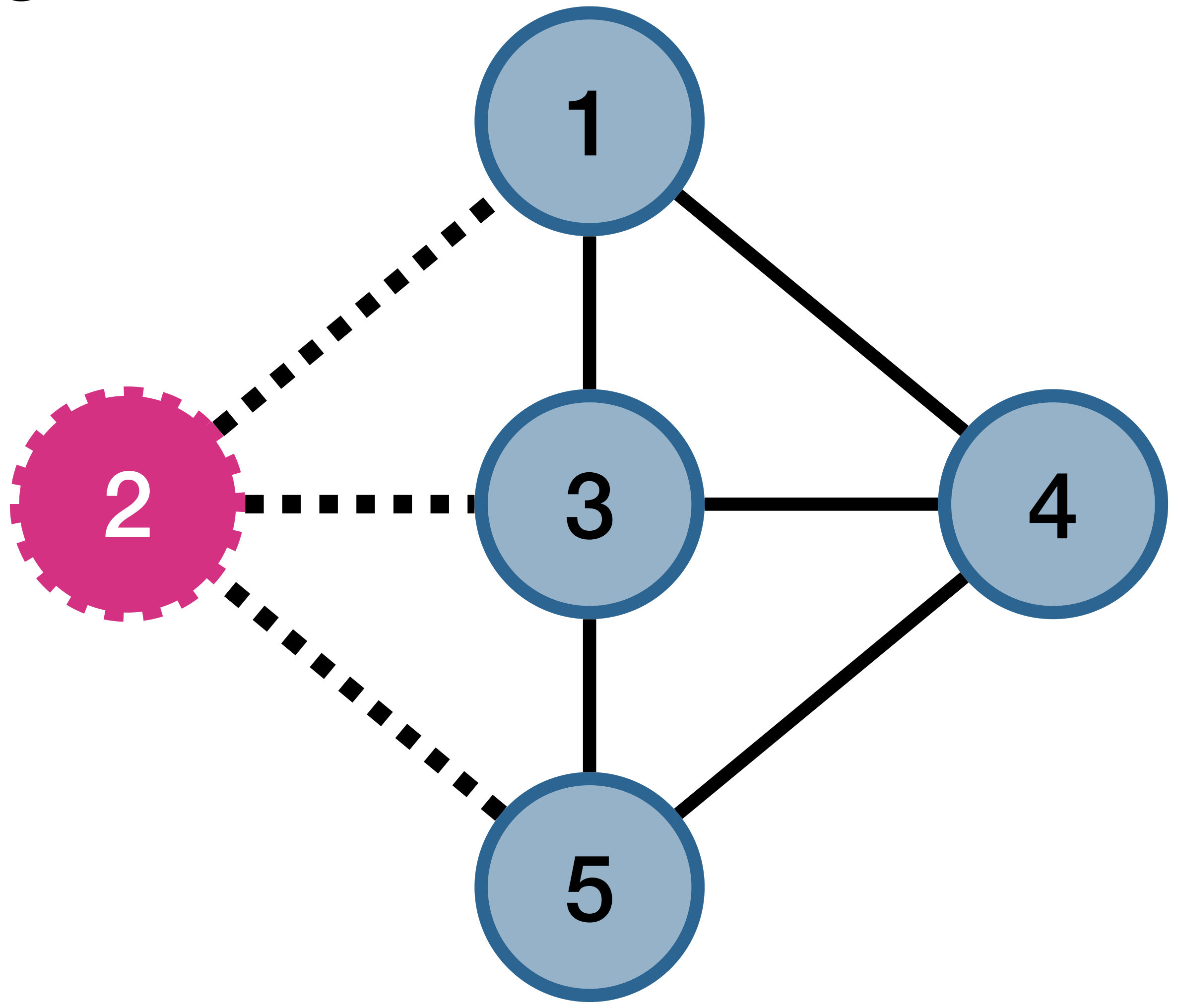
- **Expensive:** Amount of random numbers
- **Also Expensive:** Iterate over whole network in each step

SIS Simulation

naïve:



Gillespie:

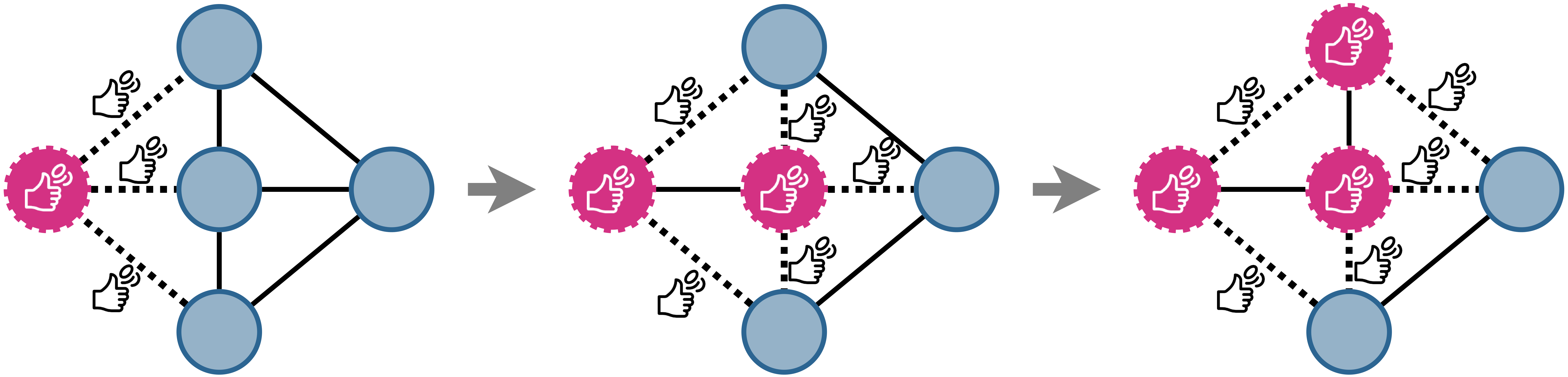


I-nodes: [2]

SI-edges [2-1, 2-3, 2-5]

SIS Simulation

naïve:



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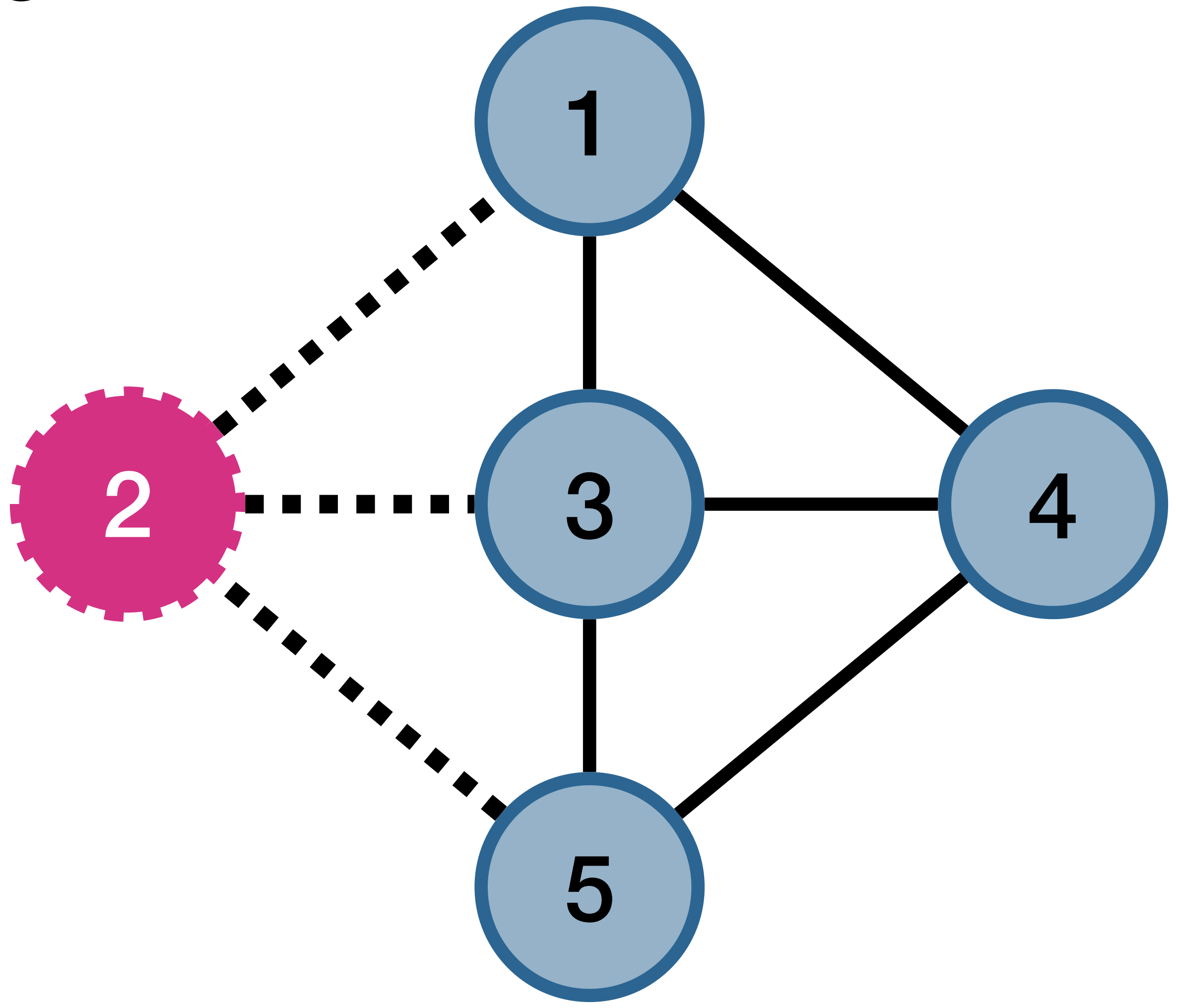

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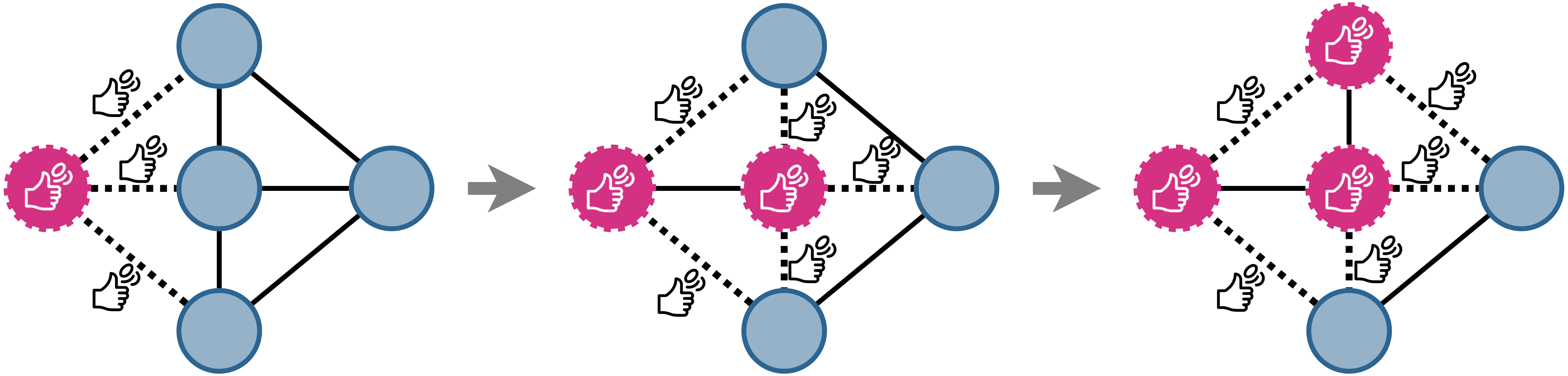
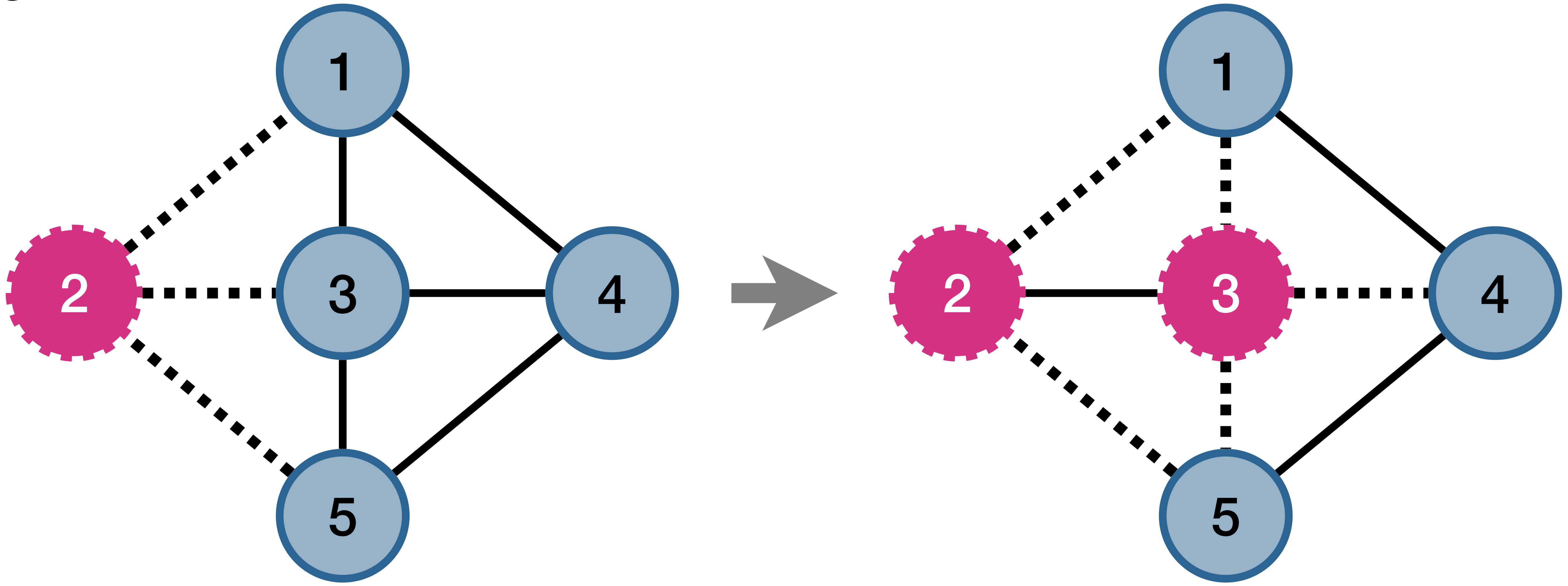


Gillespie:

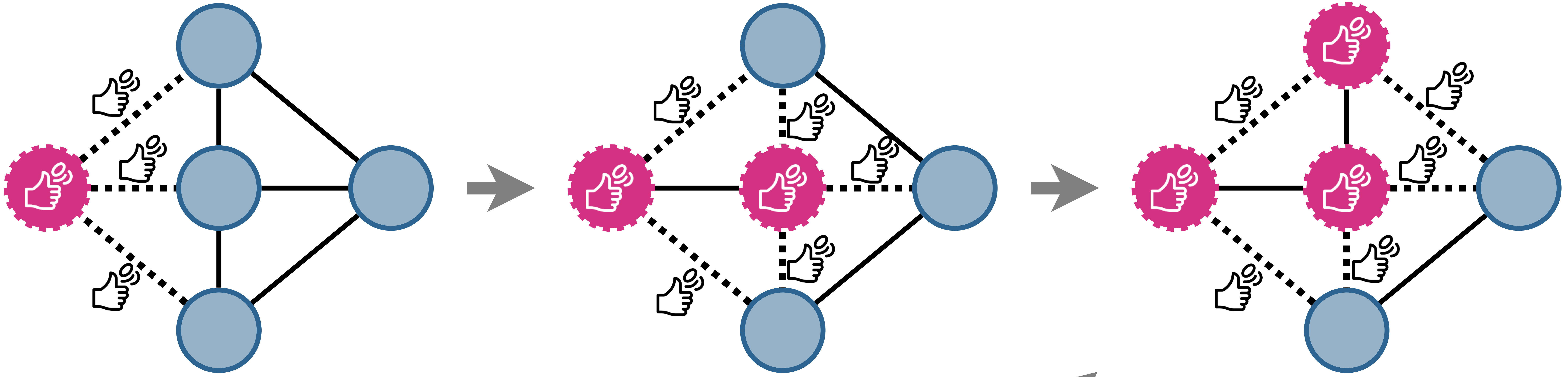


I-nodes: [2, 3]

SI-edges [2-1, 2-5, 3-1, 3-4, 3-5]

SIS Simulation

naïve:



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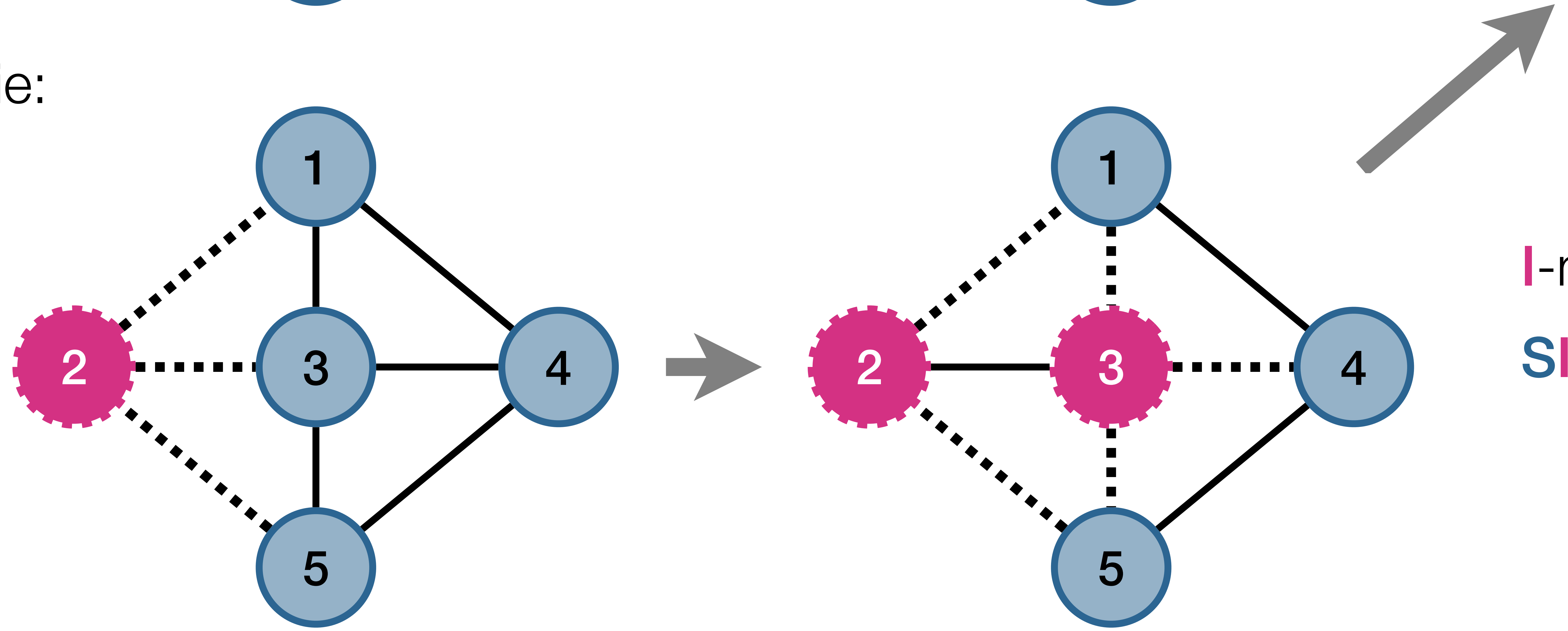

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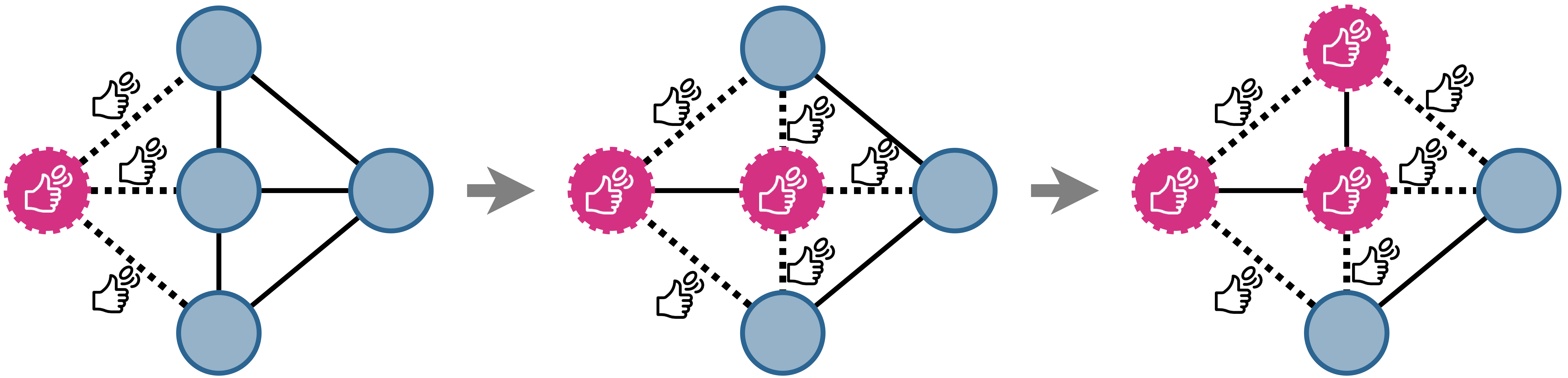
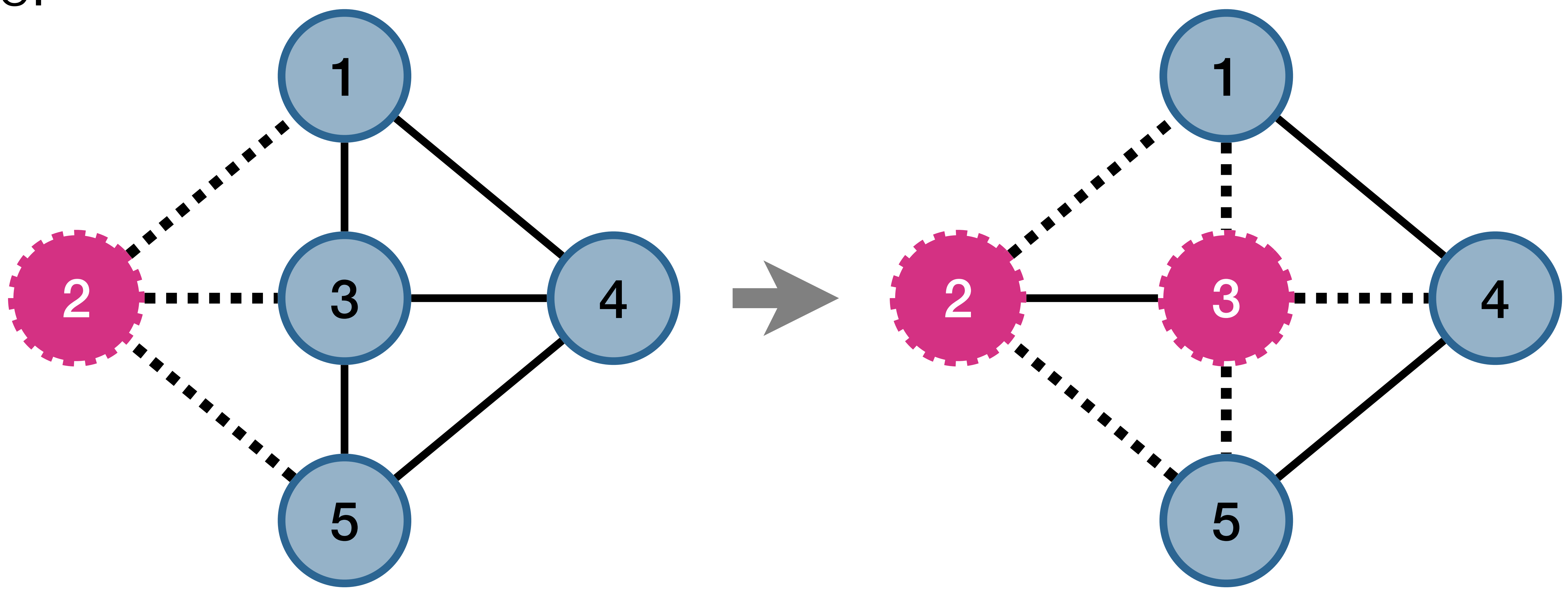


Gillespie:



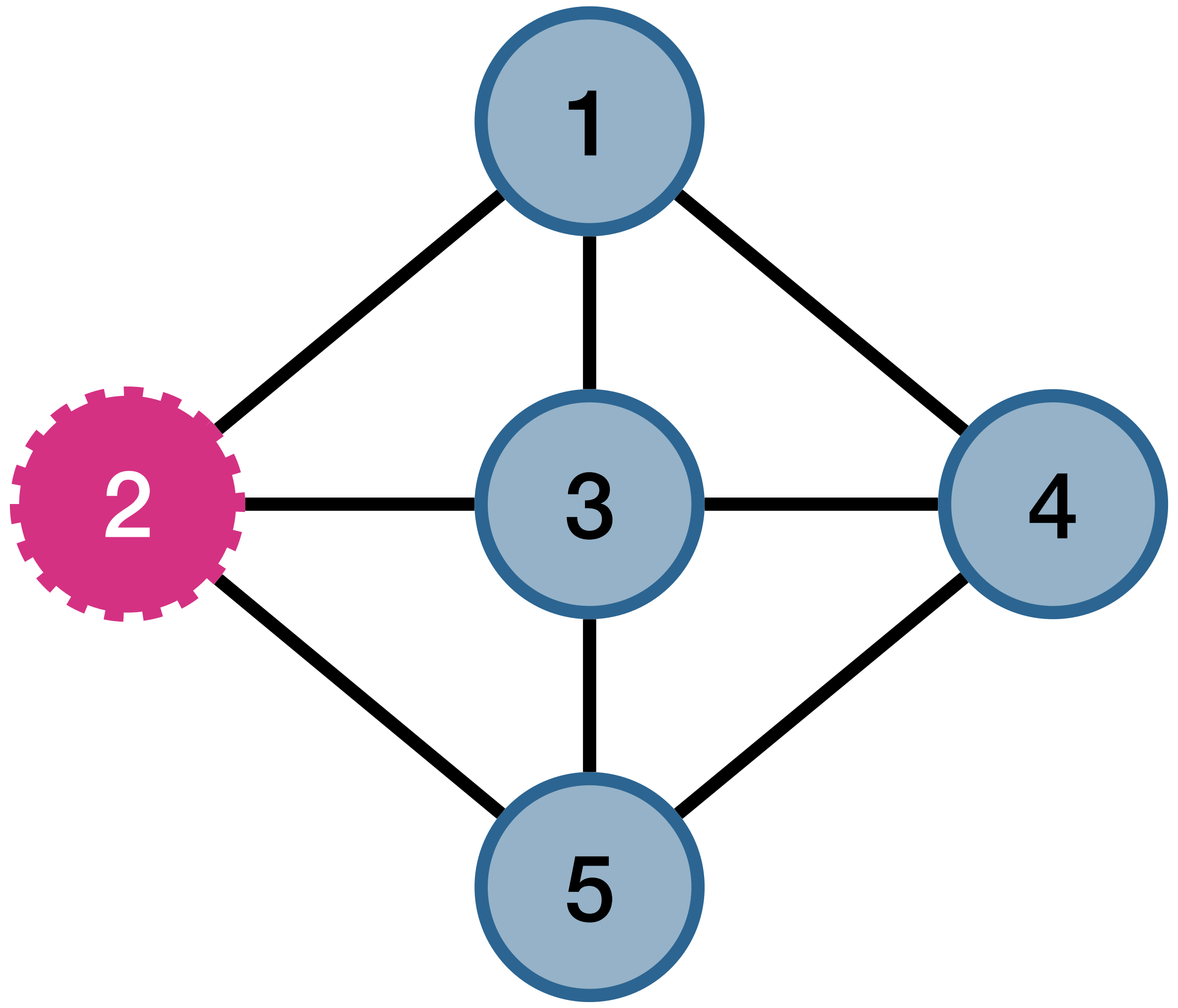
I-nodes: [2, 3]

SI-edges [2-1, 2-5, 3-1, 3-4, 3-5]

- **Cheap:** Sampling
- **Expensive:** Update lists

SIS Simulation

rejection-based:



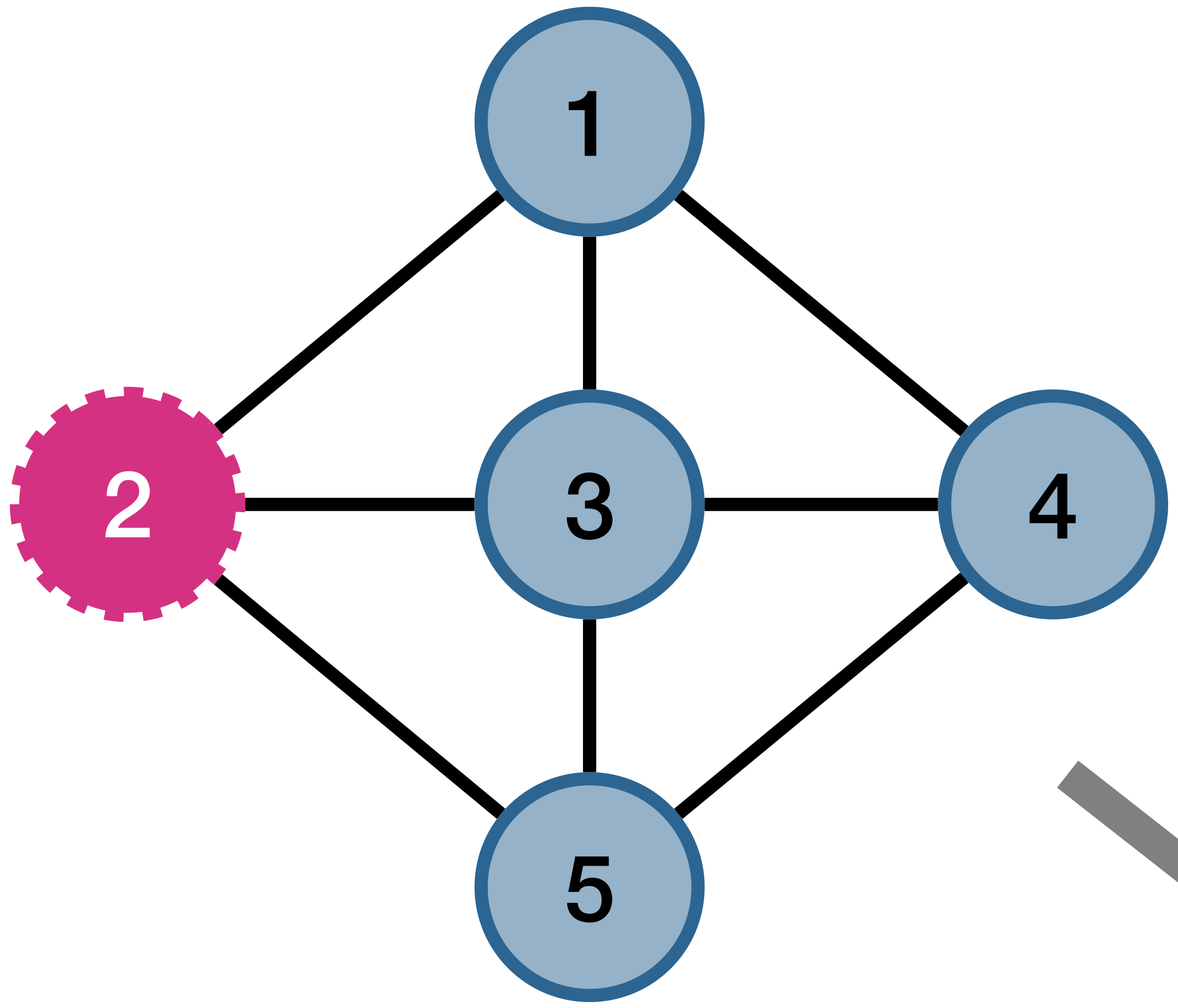
I-nodes: [2]

Sample infection source assuming **4 susceptible** neighbors

Cota and Ferreira (2017)

SIS Simulation

rejection-based:



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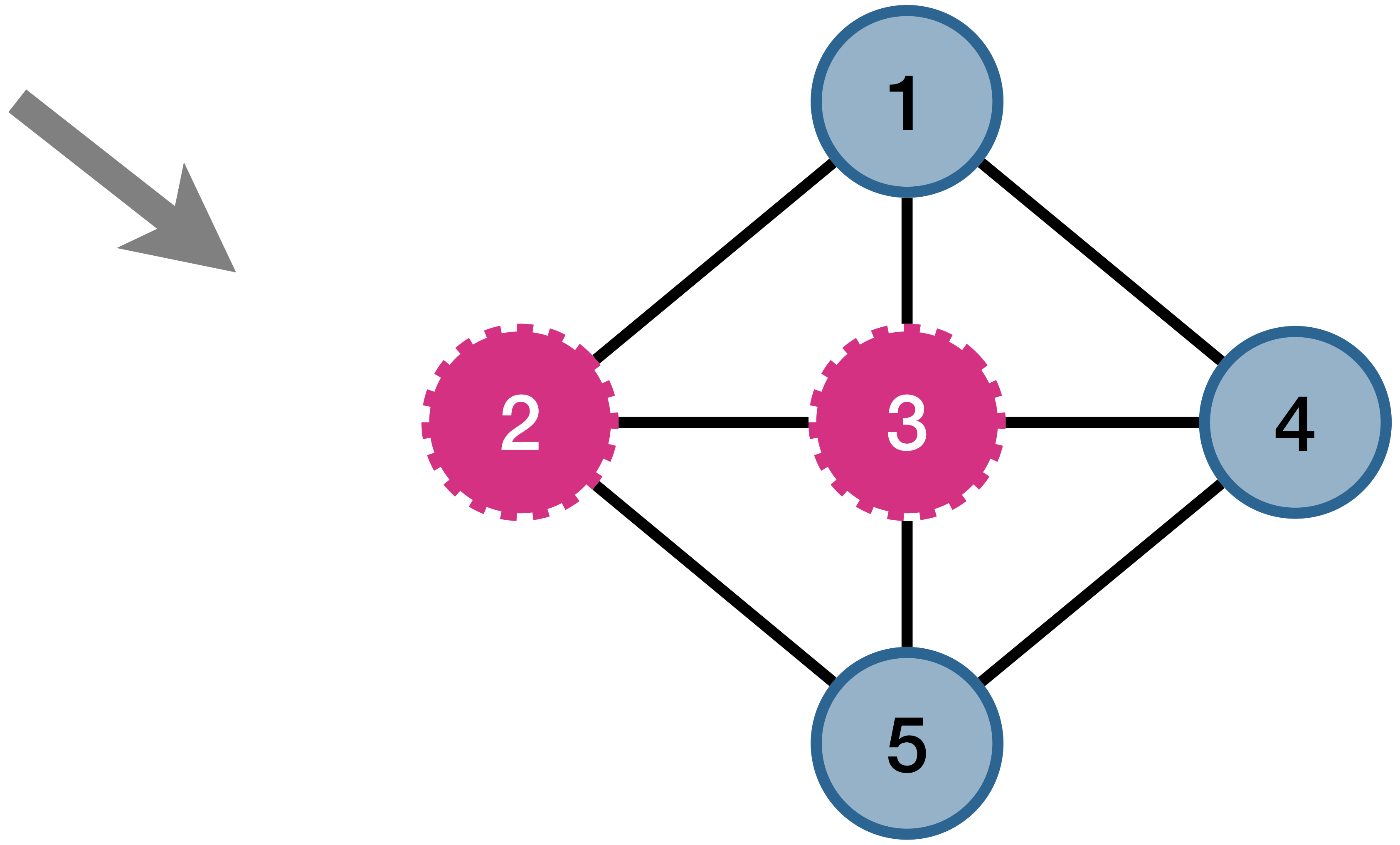
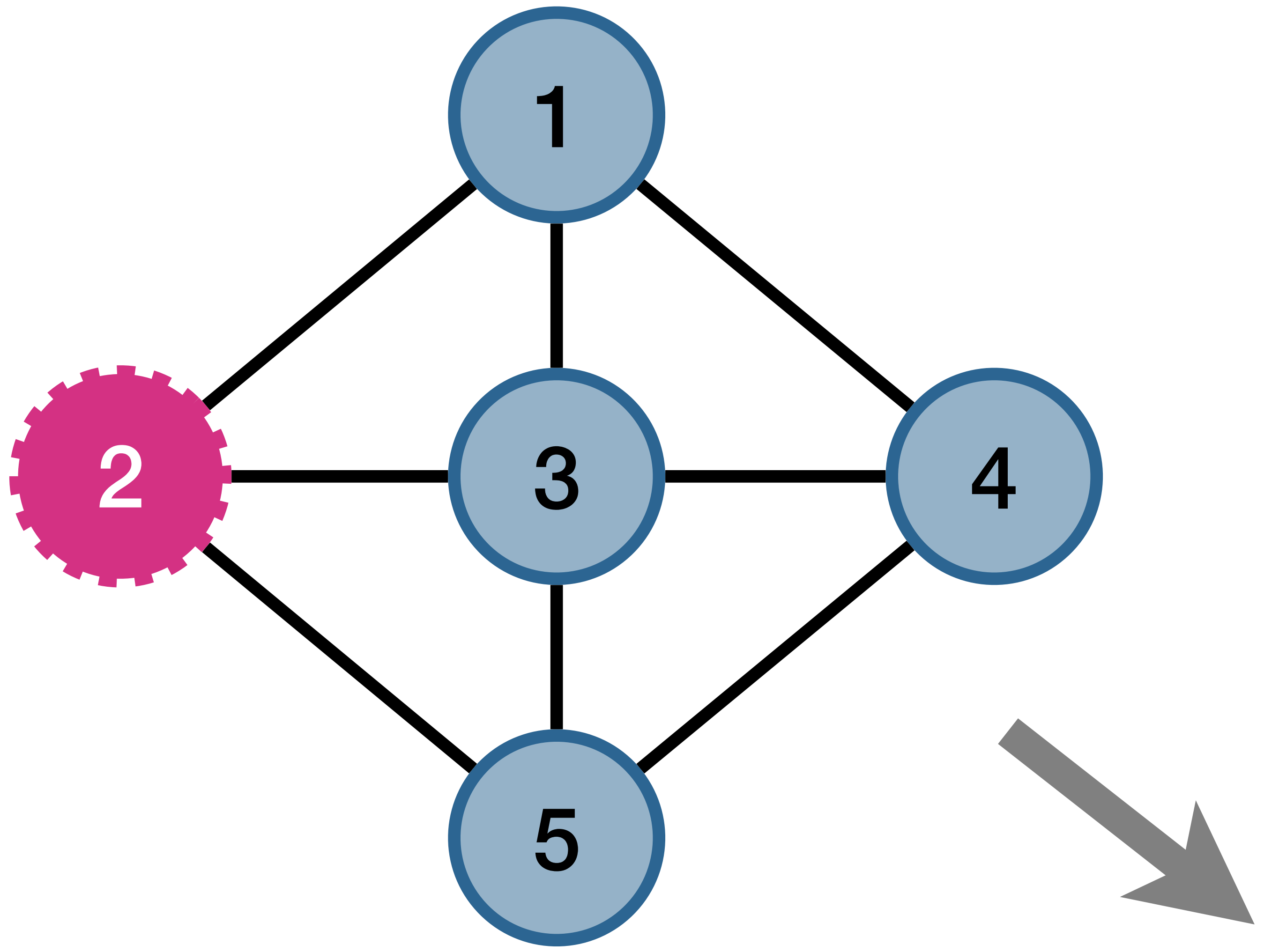


rejection probability
= **25%**

Cota and Ferreira (2017)

SIS Simulation

rejection-based:



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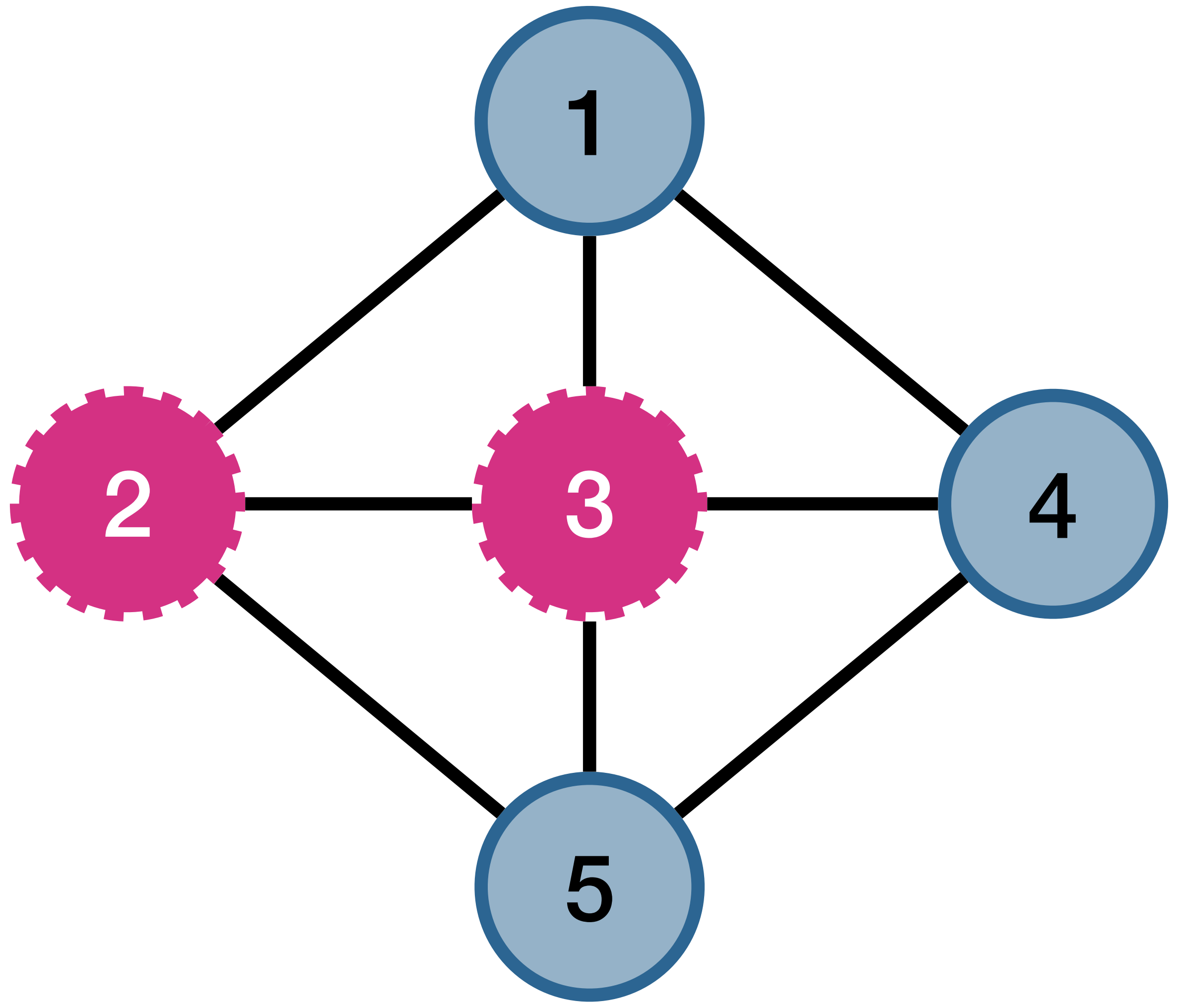

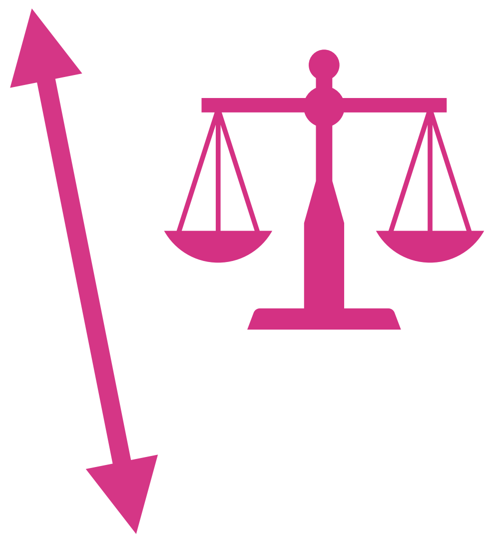

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SIS Simulation

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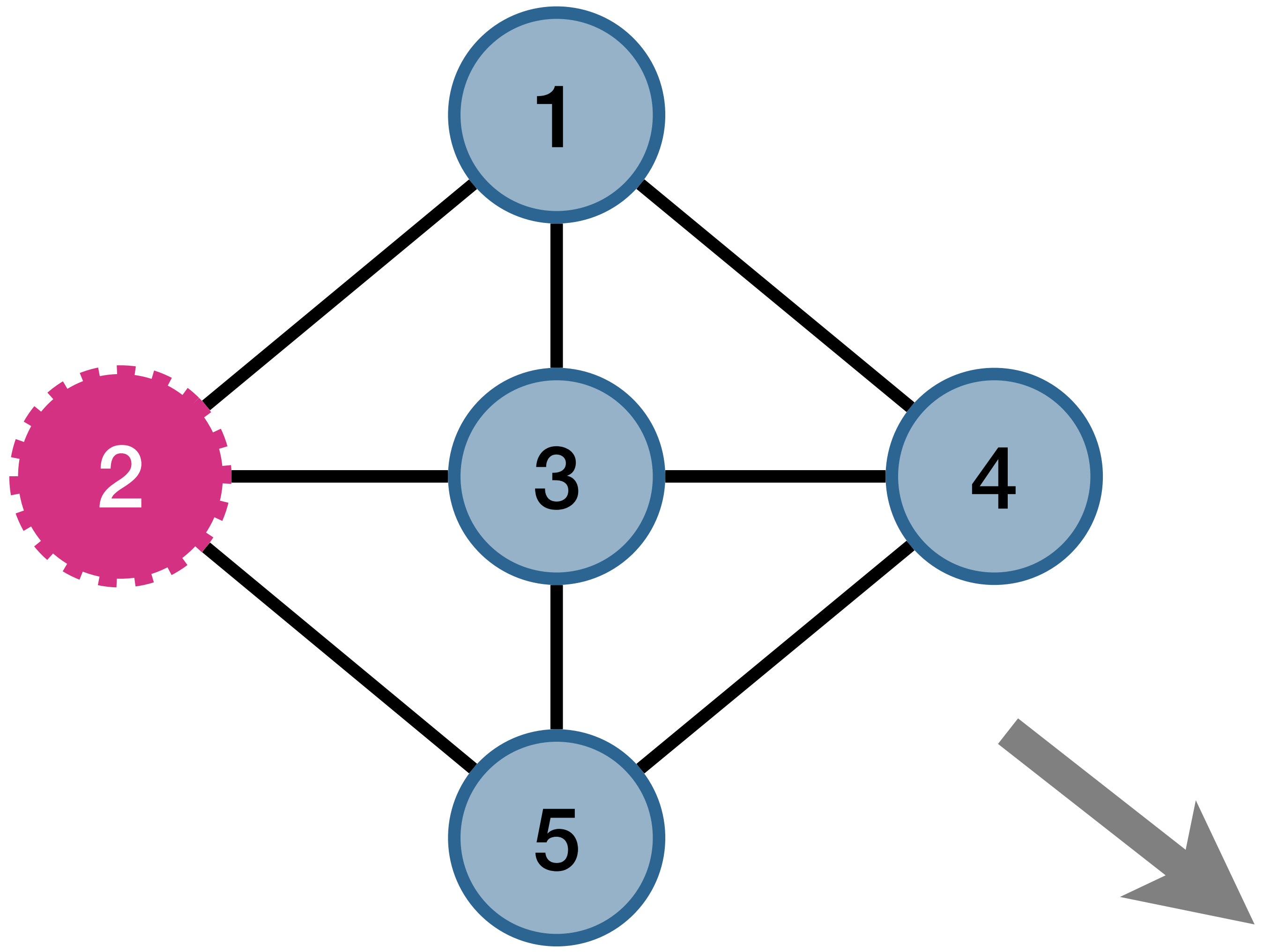

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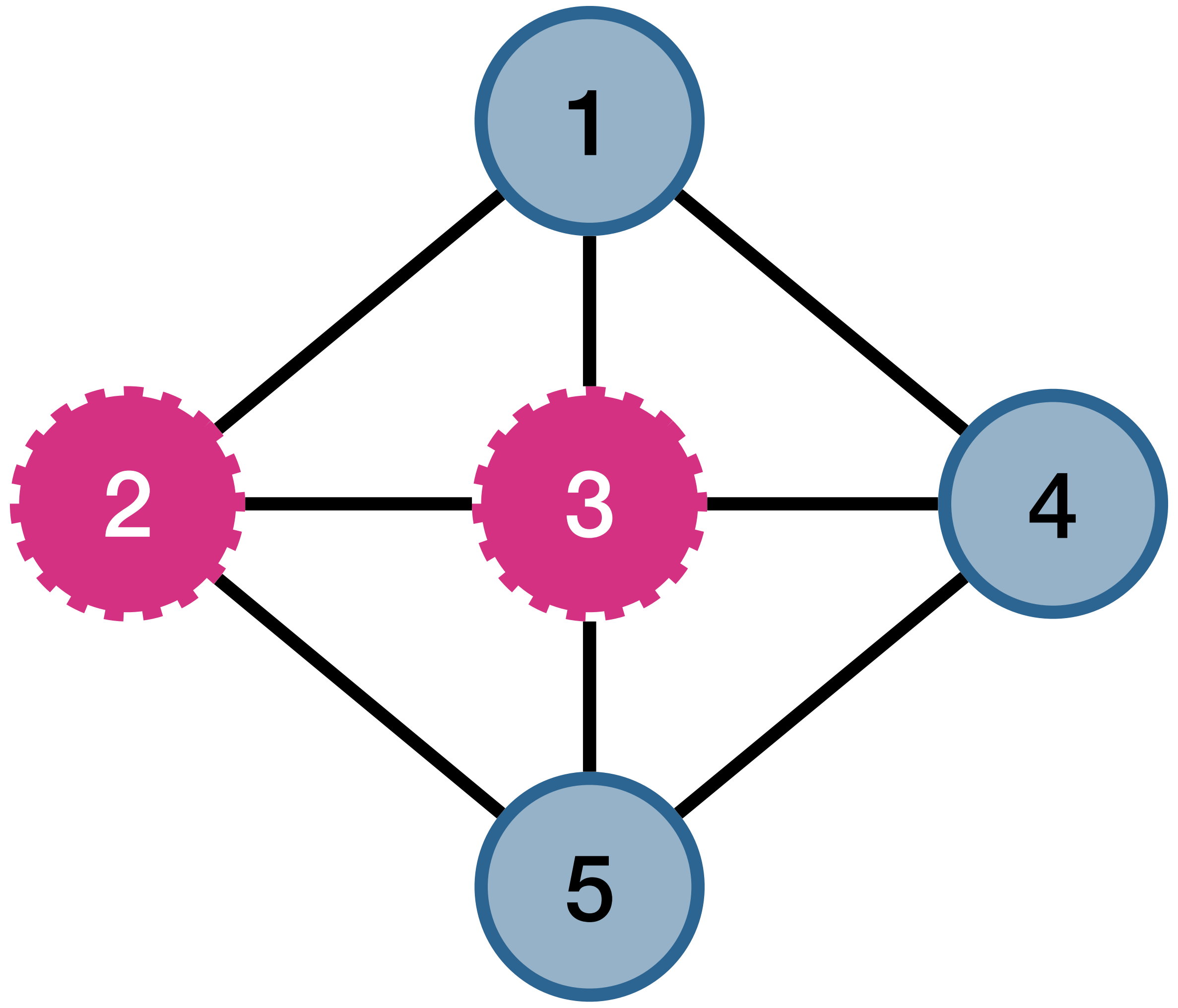
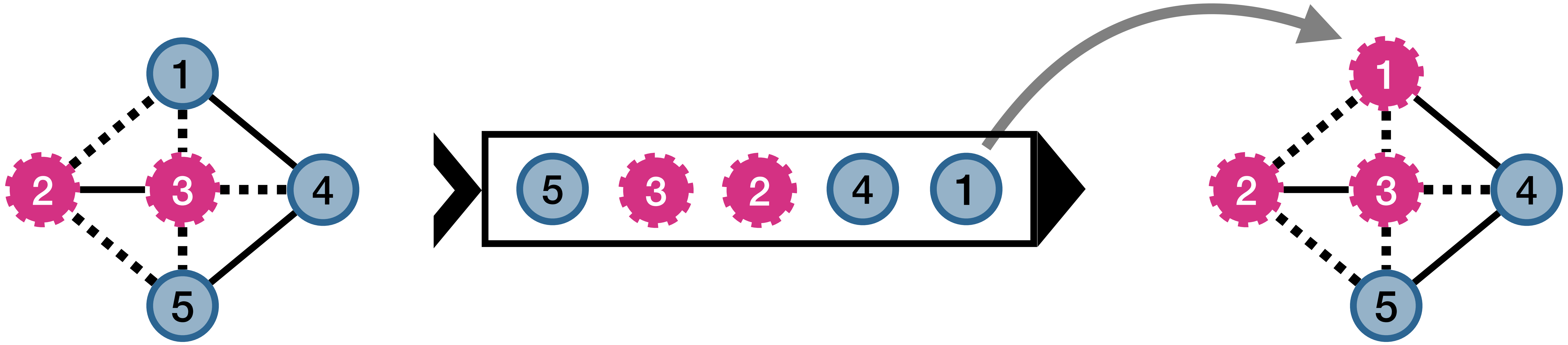


- **Cheap:** Sampling
- **Also cheap:** Update lists
- **Expensive:** Amount of rejections

Cota and Ferreira (2017)

Event-Driven Simulation

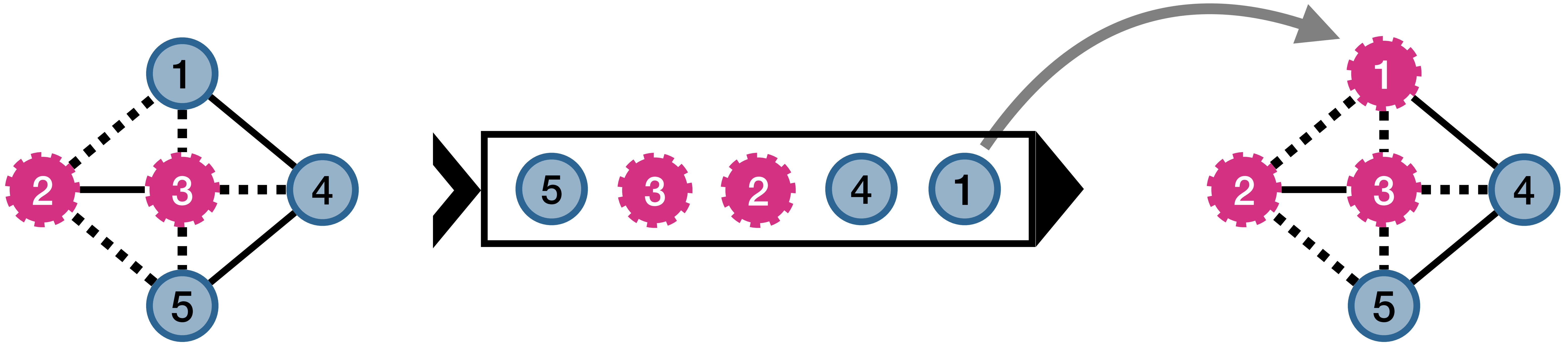
event-driven:



1. Pop event.
2. Update node.
3. Create new event.
4. Update neighborhood.

Event-Driven Simulation

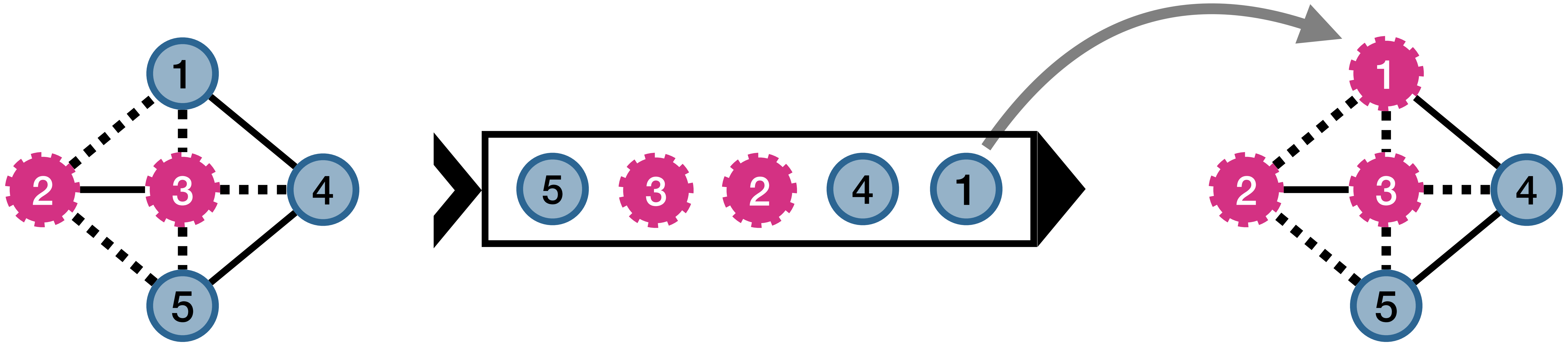
event-driven:



1. Pop event.
2. Update node.
3. Create new event.
4. Update neighborhood (expensive).

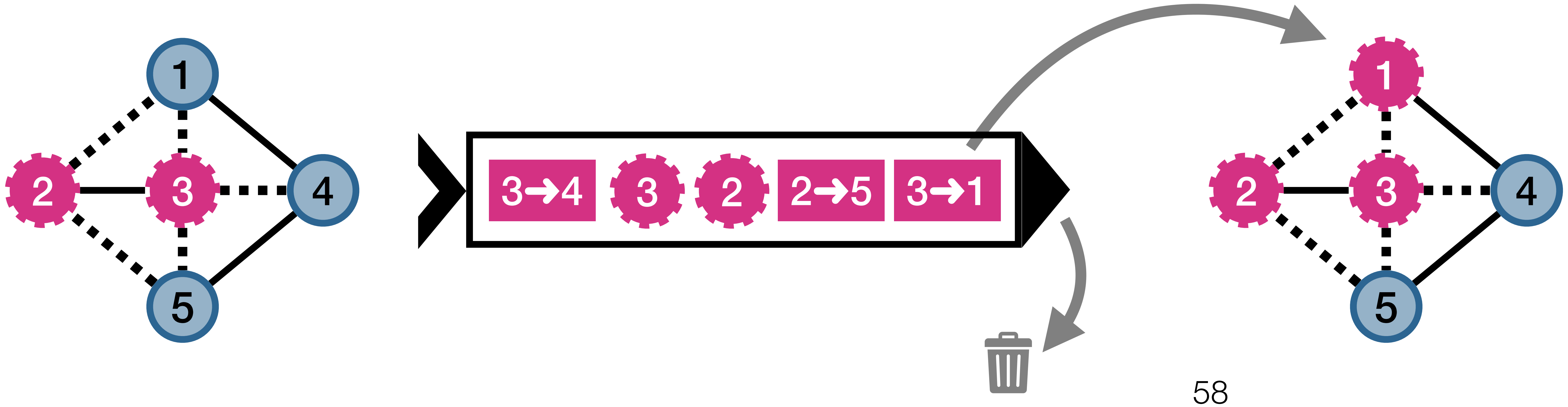
Our Method

event-driven:



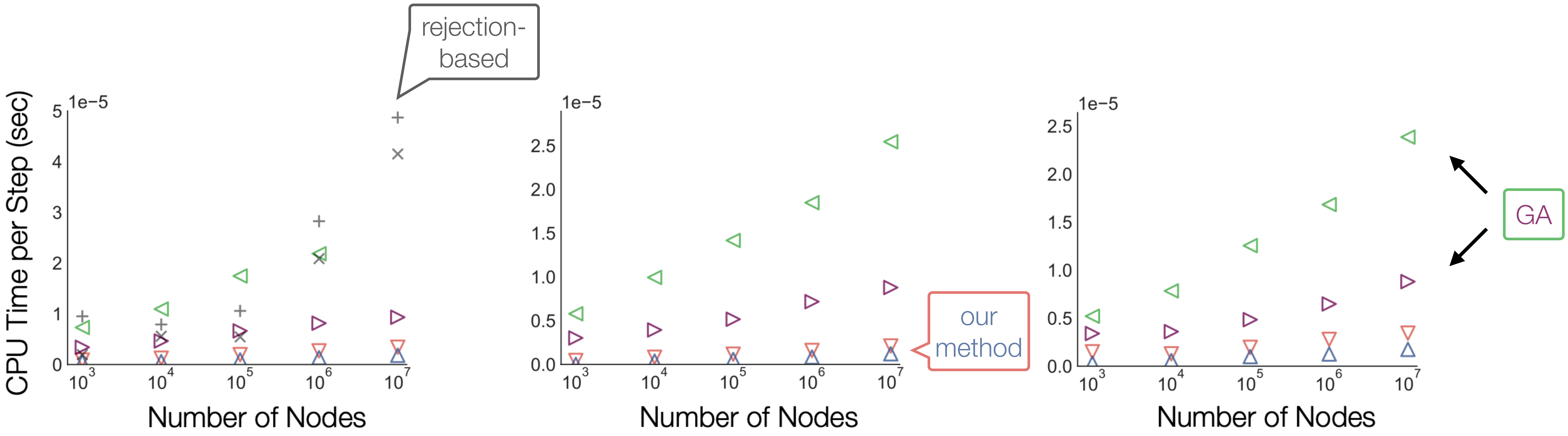
1. Pop event.
2. Update node.
3. Create new event.
4. Update neighborhood (expensive).

rejection-based + event-driven (our method):



1. Pop event (possible rejection).
2. Update node.
3. Create new event (possible rejection).
4. ~~Update neighborhood.~~

SIS Simulation: Results

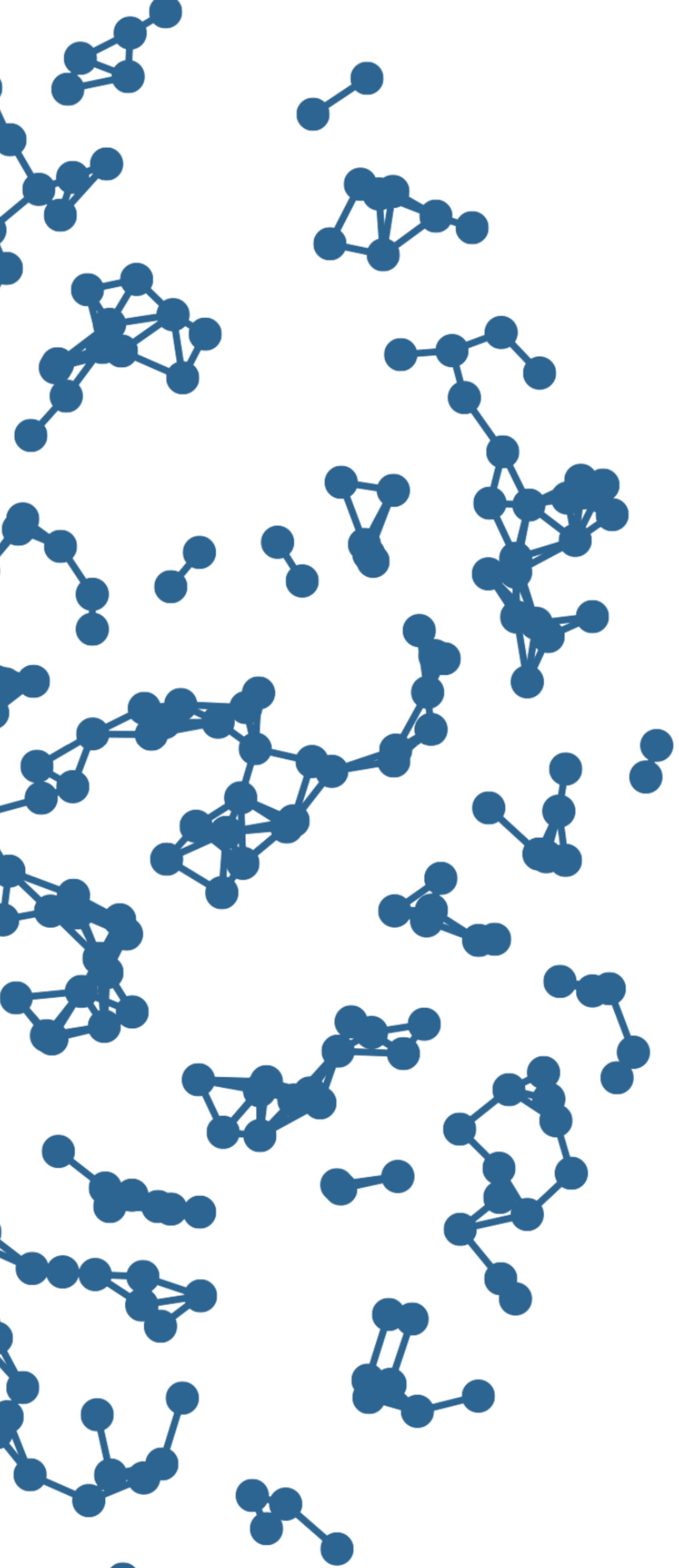


SIS

SIRS

SIJS

(competing pathogens)



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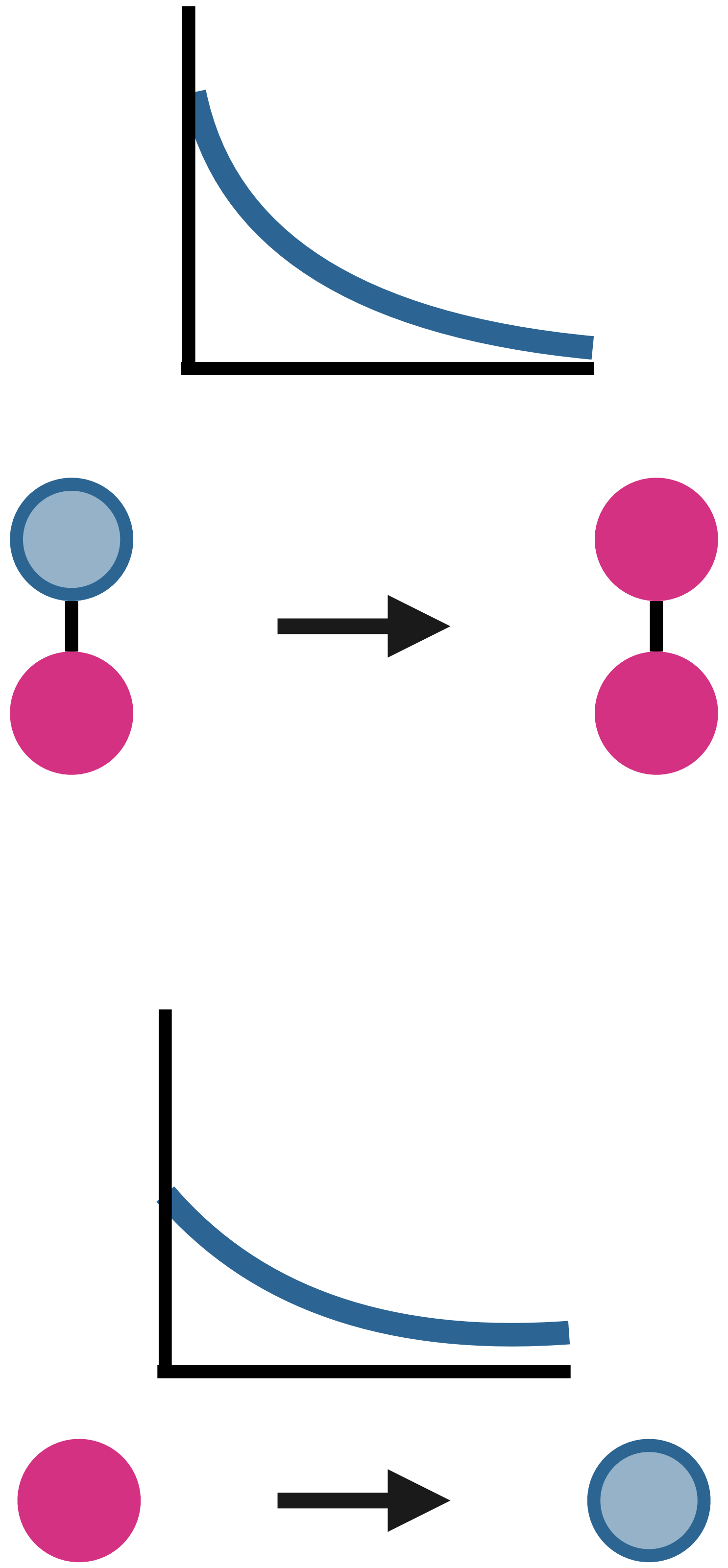
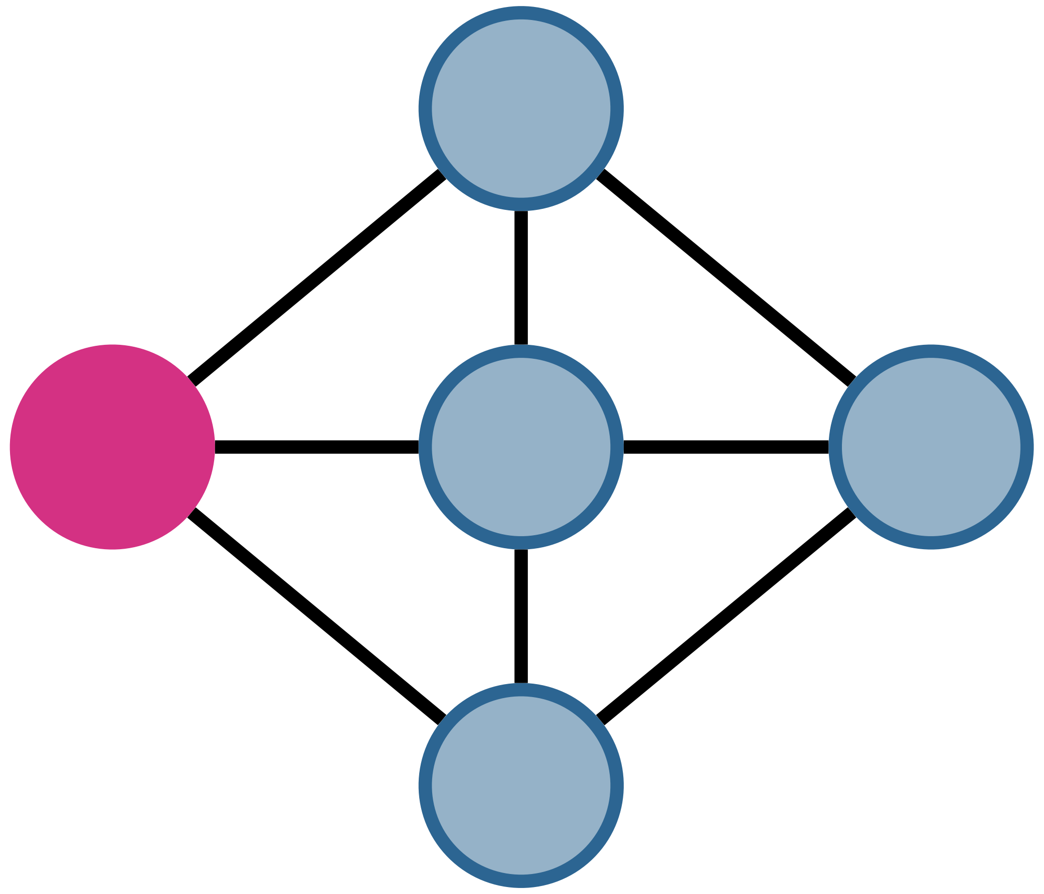
Non-Markovian Models

Markovian:

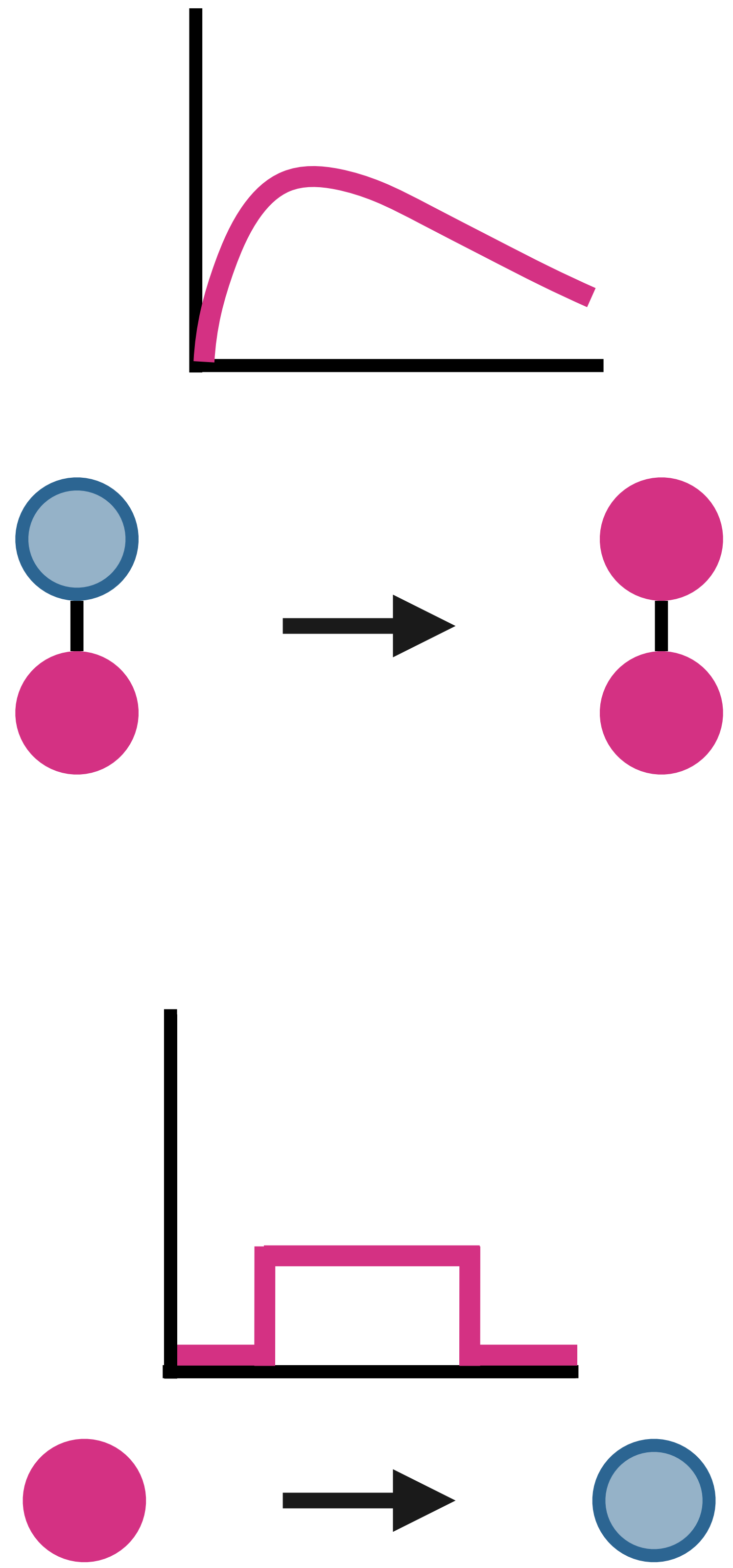


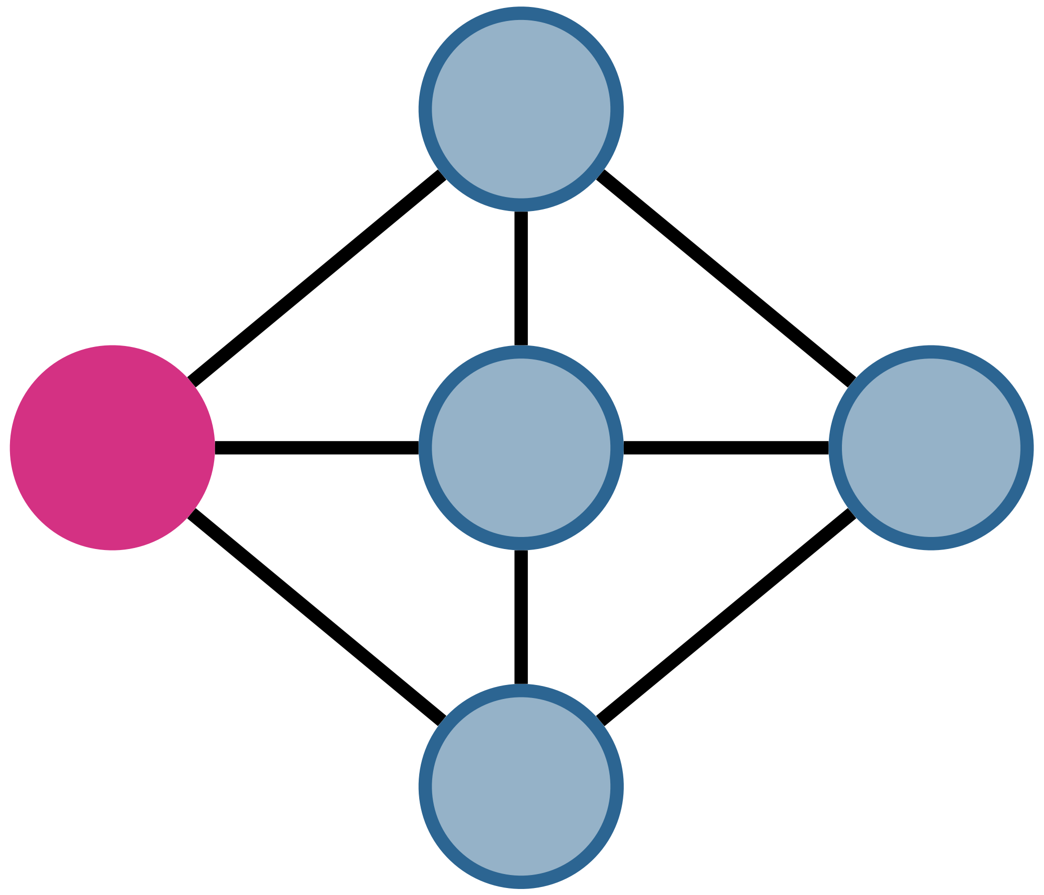


- **Trade-off:** simplicity vs accuracy
- Vastly different properties
- Difficult to analyse

Non-Markovian Models

Non-Markovian:





- **Trade-off:** simplicity vs accuracy
- Vastly different properties
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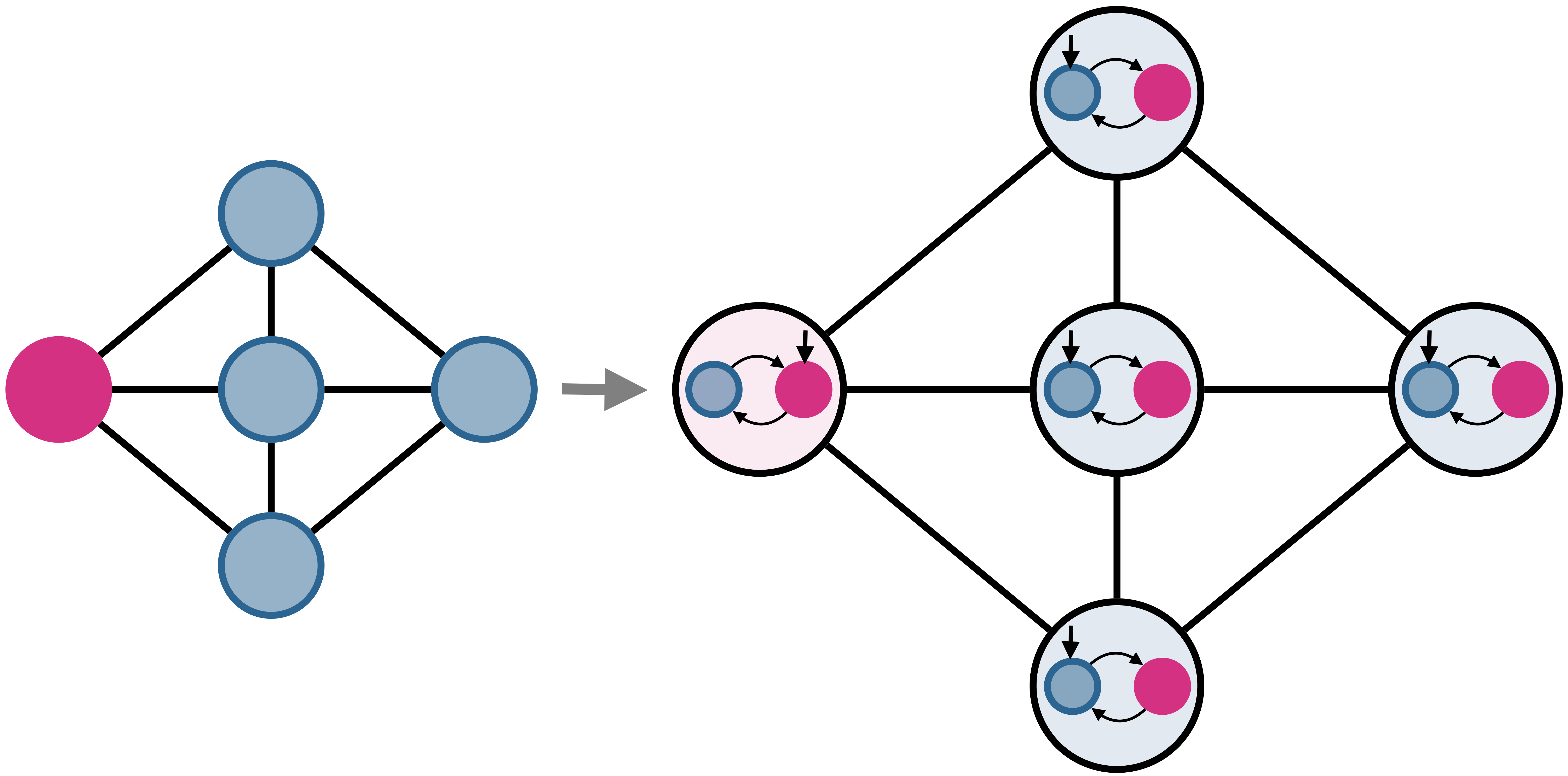
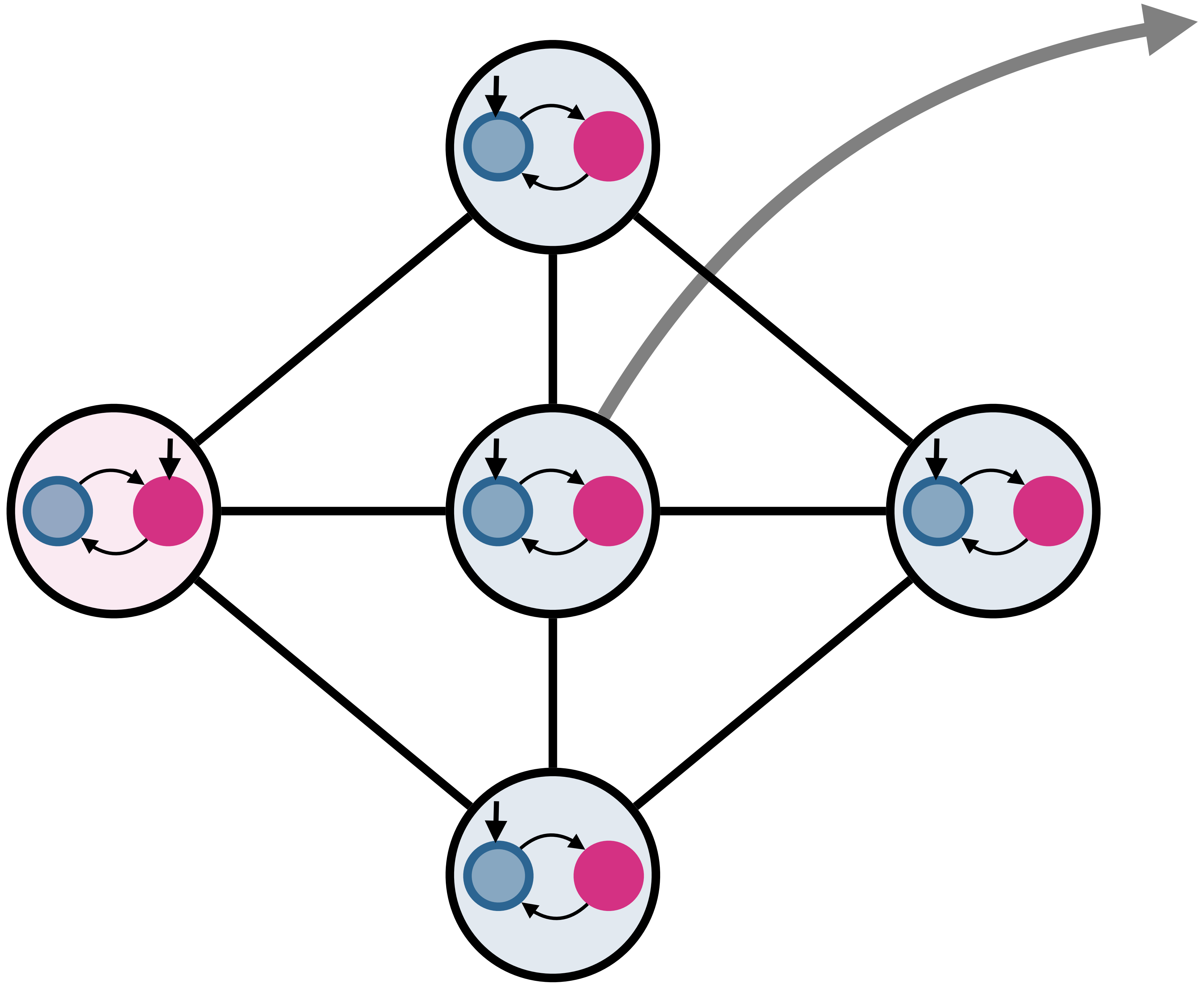
Non-Markovian Models

Goal: Universal framework for non-Markovian dynamical systems

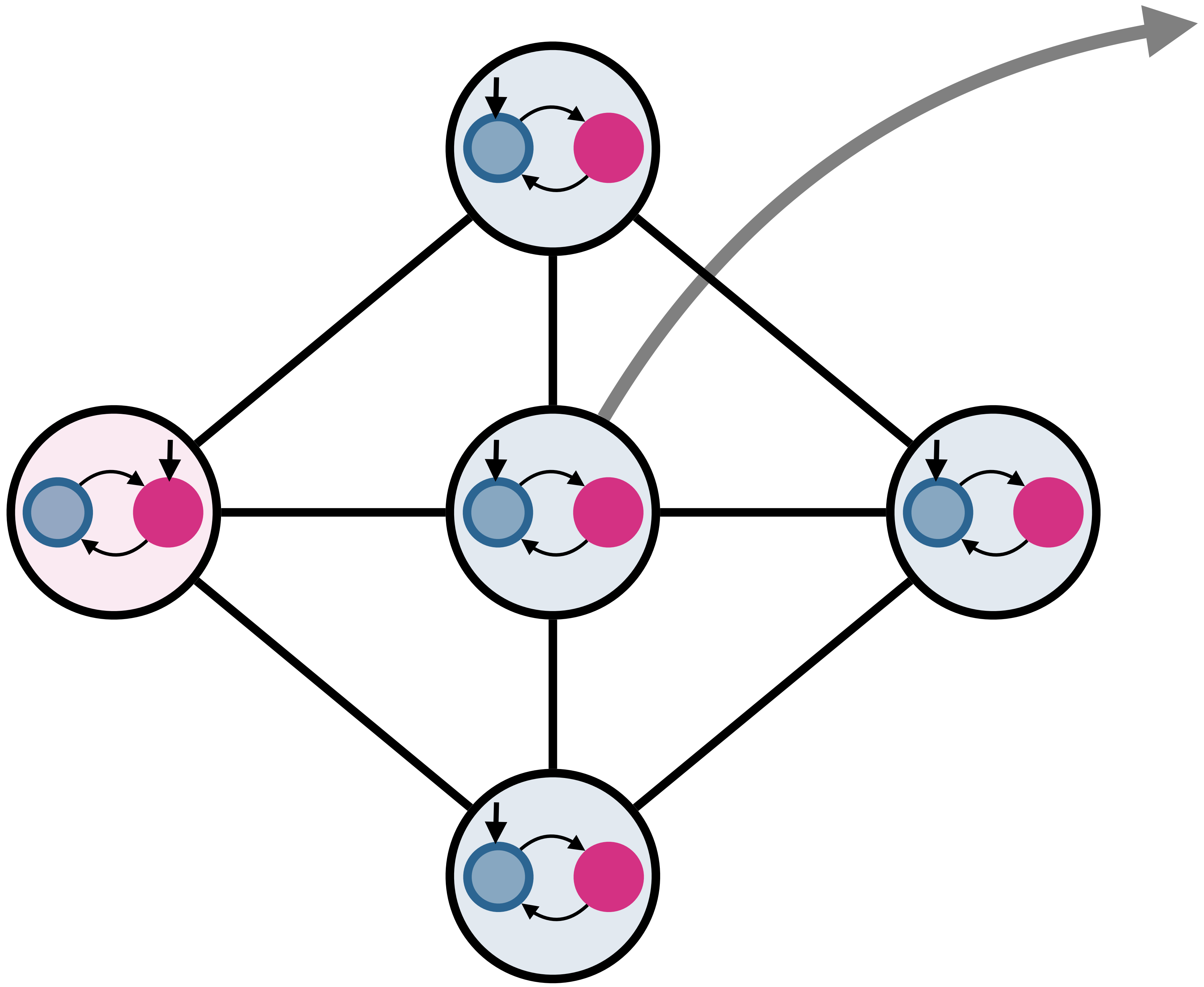


Non-Markovian Models



- Agent-specific rate function
- Changes continuously in time.
- Depends on Markov blanket.

Non-Markovian Models

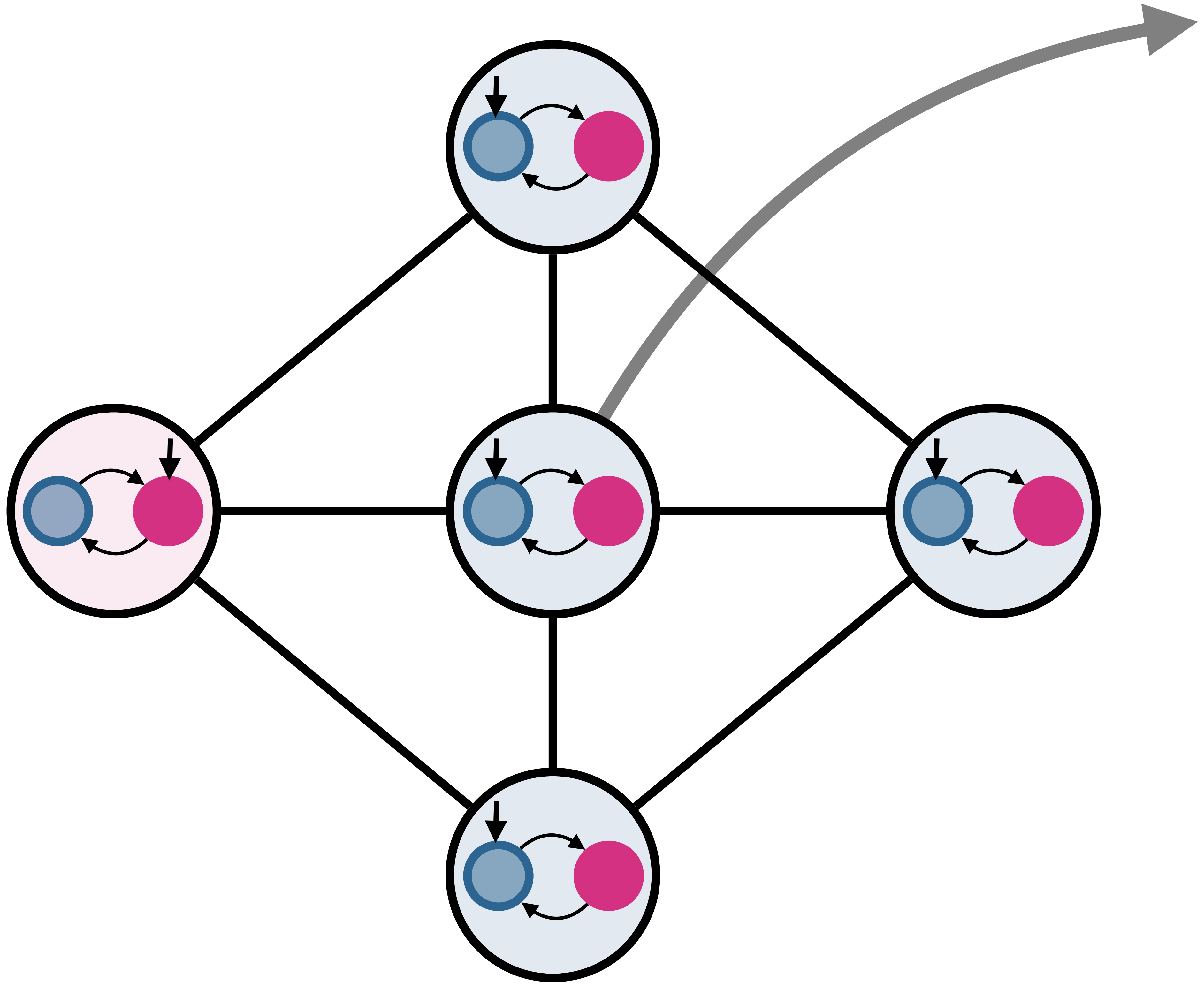


Input:

- Current state:
- Residence time: 0.42
- State and residence time of all neighbors:

$\{(\;,0.1)$
$(\;,2.7)$
$(\;,1.5)$
$(\;,0.2)\}$

Non-Markovian Models



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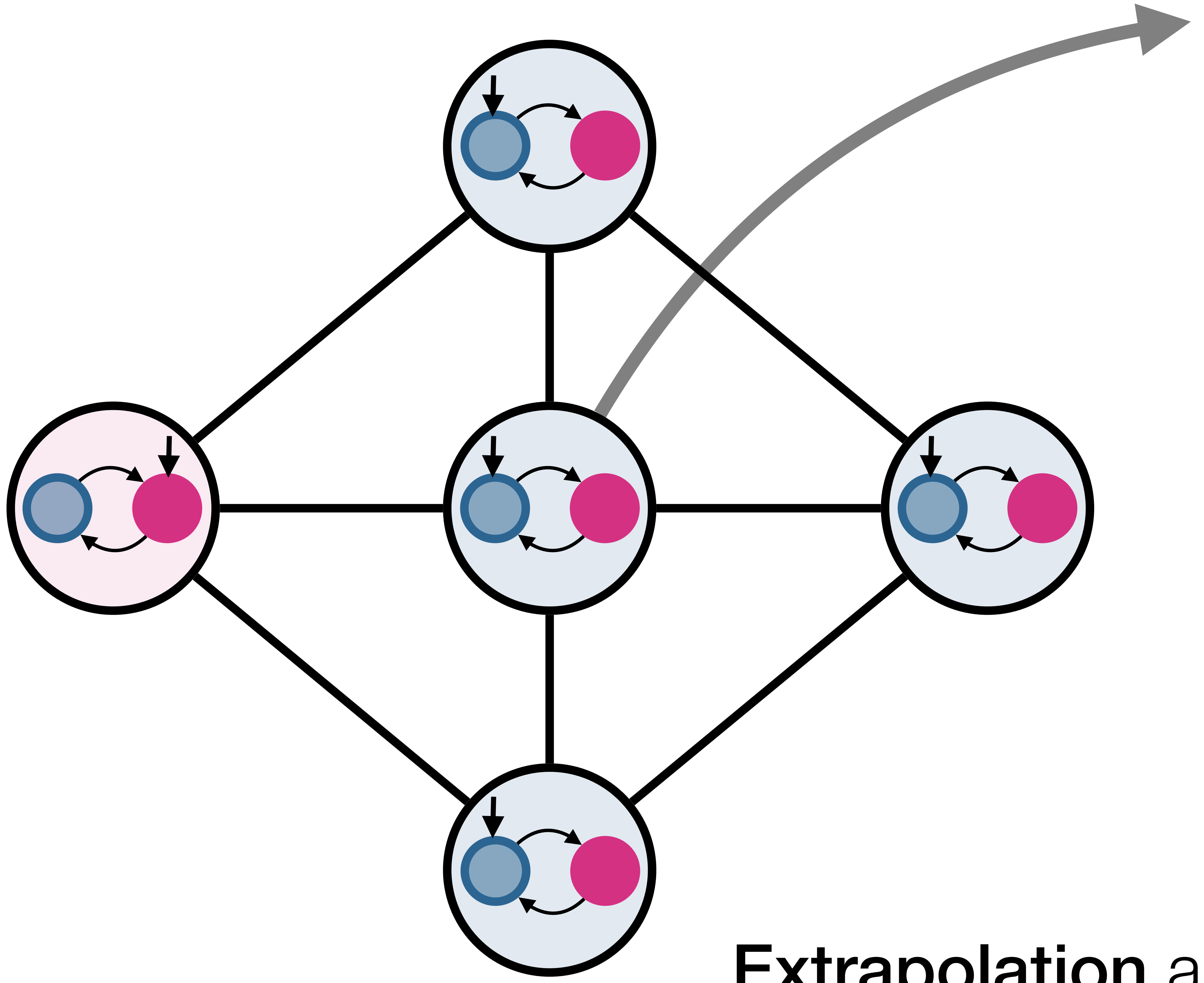
$\{(\;,0.1)$
$(\;,2.7)$
$(\;,1.5)$
$(\;,0.2)\}$

Output:

- Next state
- Instantaneous rate: 1.5

Non-Markovian Models

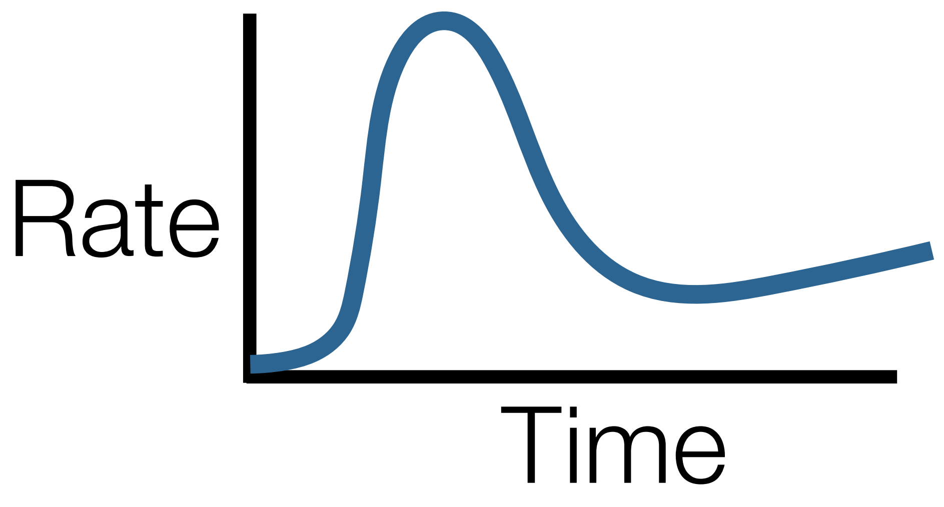


Input:

- Current state:
- Residence time: 0.42
- State and residence time of all neighbors:

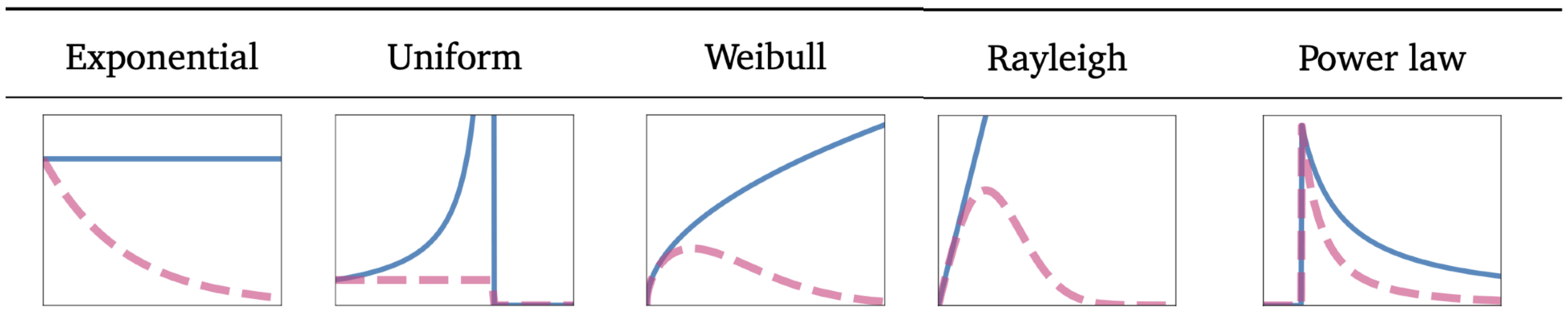
$$\{(\ ,0.1)\ (\ ,2.7)\ (\ ,1.5)\ (\ ,0.2)\}$$

Extrapolation assuming fixed neighborhood:



Non-Markovian Simulation

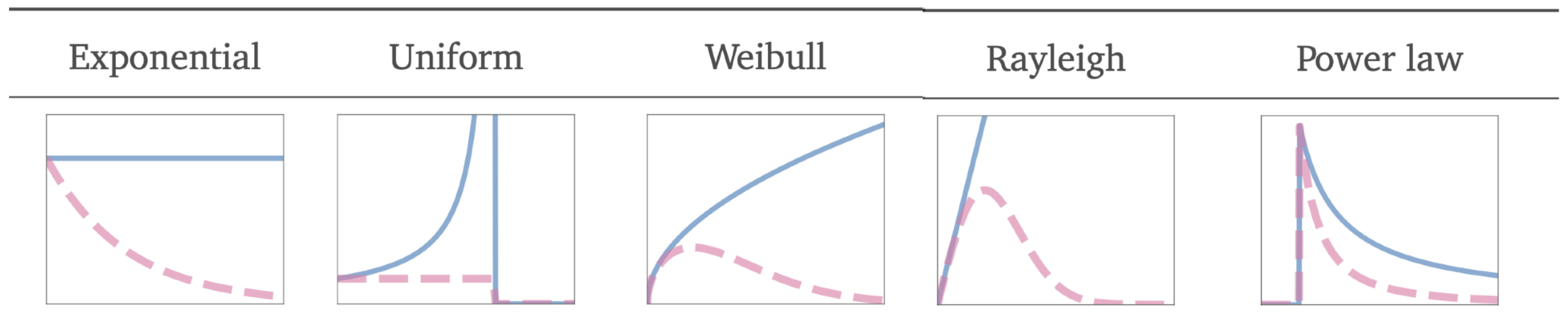
Rate functions are universal:



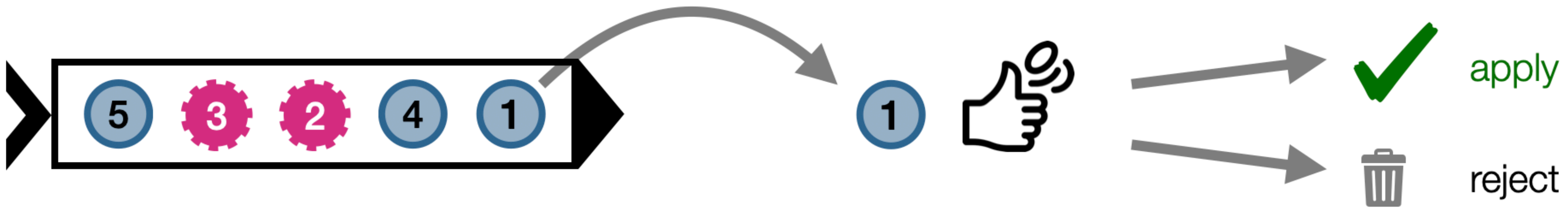
- Time-dependent rate function
- Jump-time probability density

Non-Markovian Simulation

Rate functions are universal:



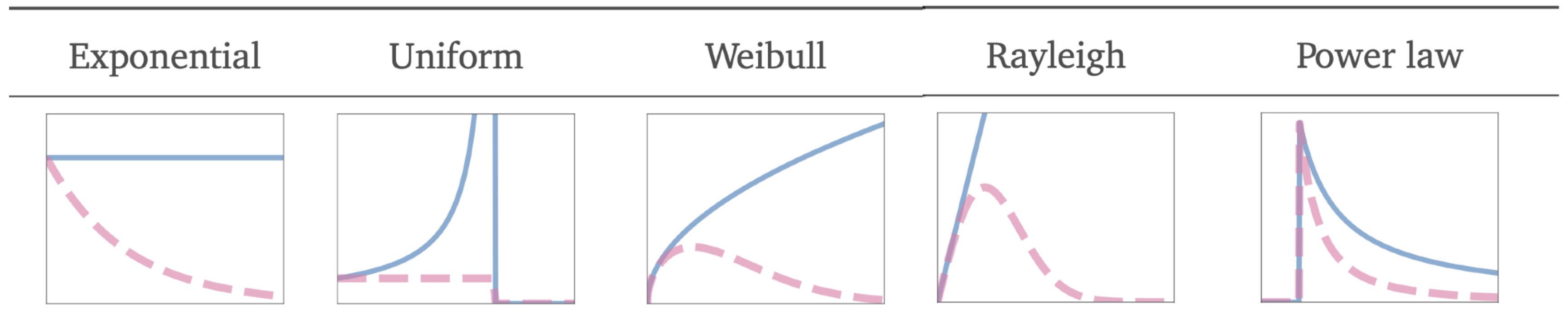
Over-approximations can be balanced out with rejections.



1. Pop event (possible rejection).
2. Update agent.
3. Create new event.
4. ~~Update neighborhood.~~

Non-Markovian Results

Rate functions are universal:



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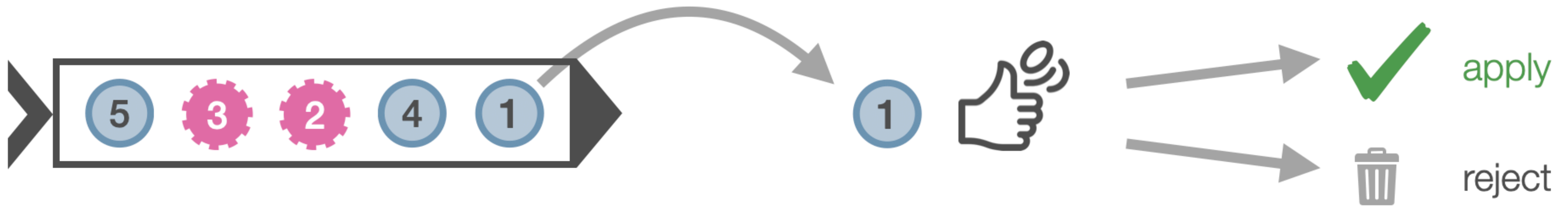

1. Pop event (possible rejection).
2. Update agent.
3. Create new event.
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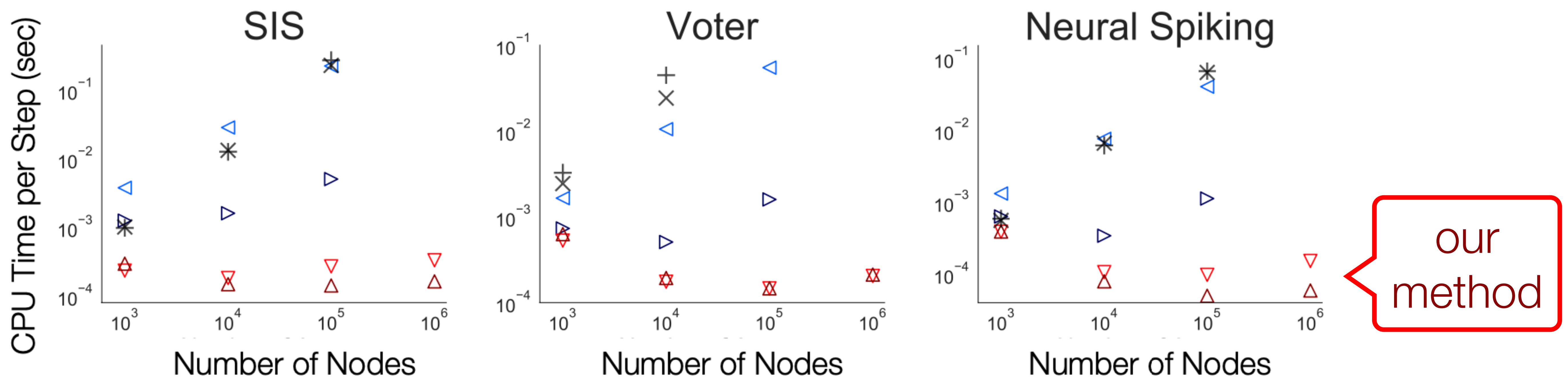
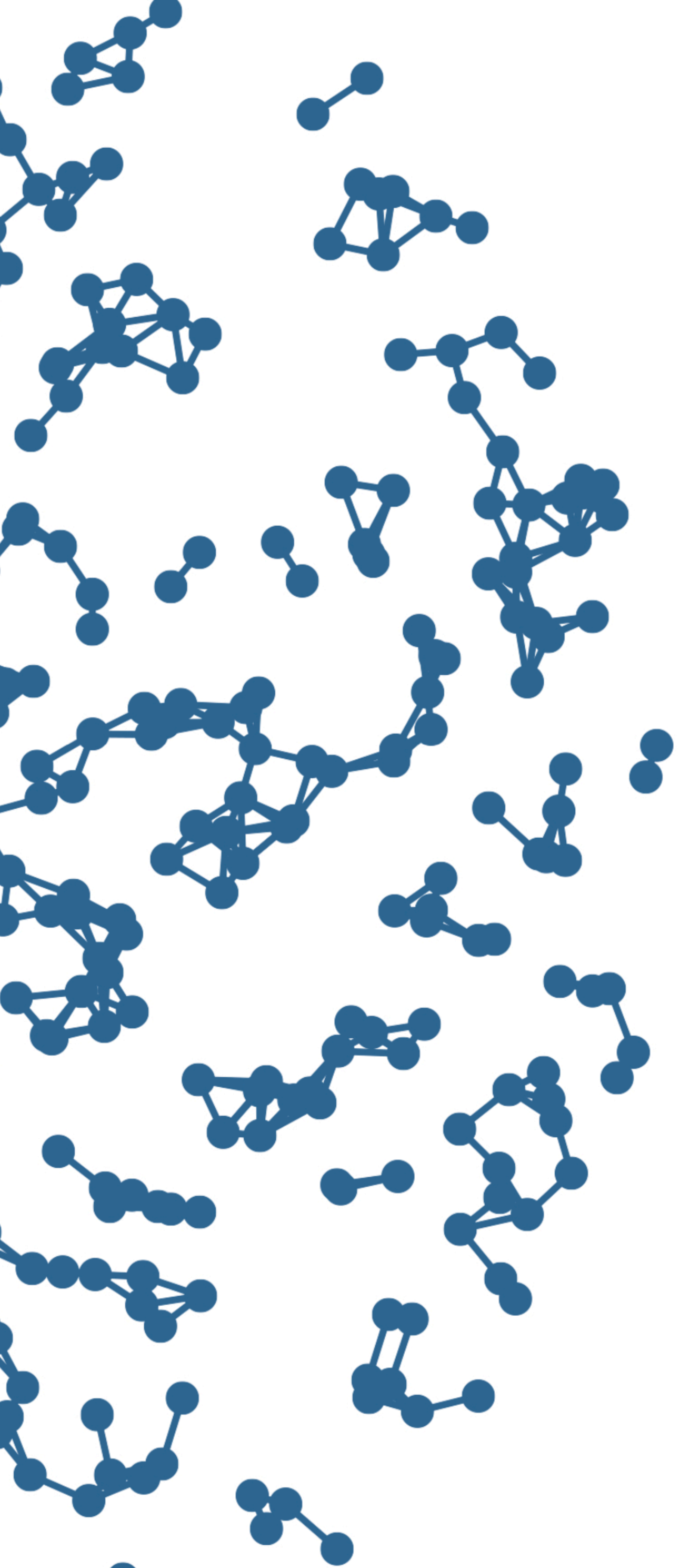
Results:



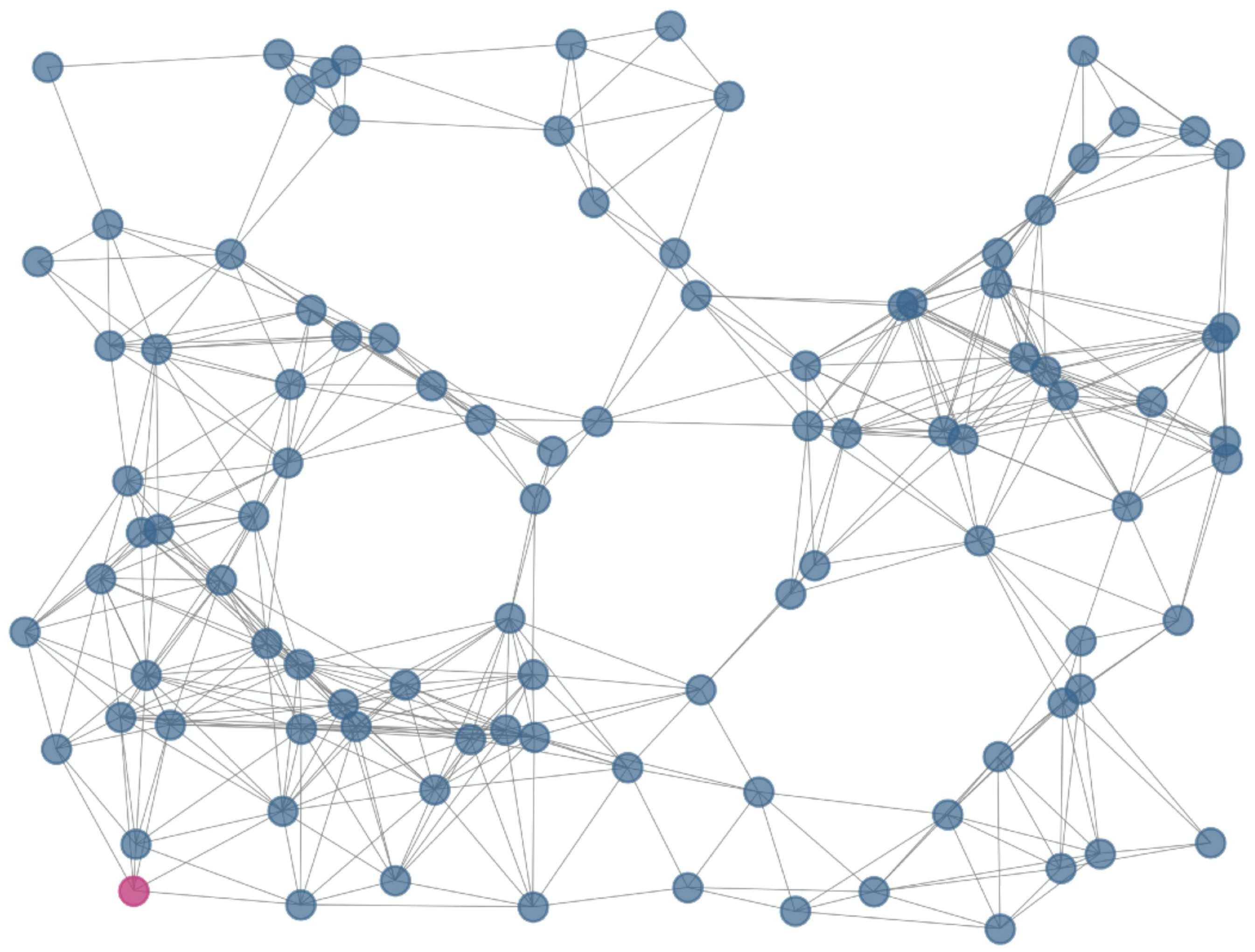


Agenda

METHODS

COVID
(NON-)MARKOVIAN SIMULATION
CONTROL
INFERENCE

Problem Setting



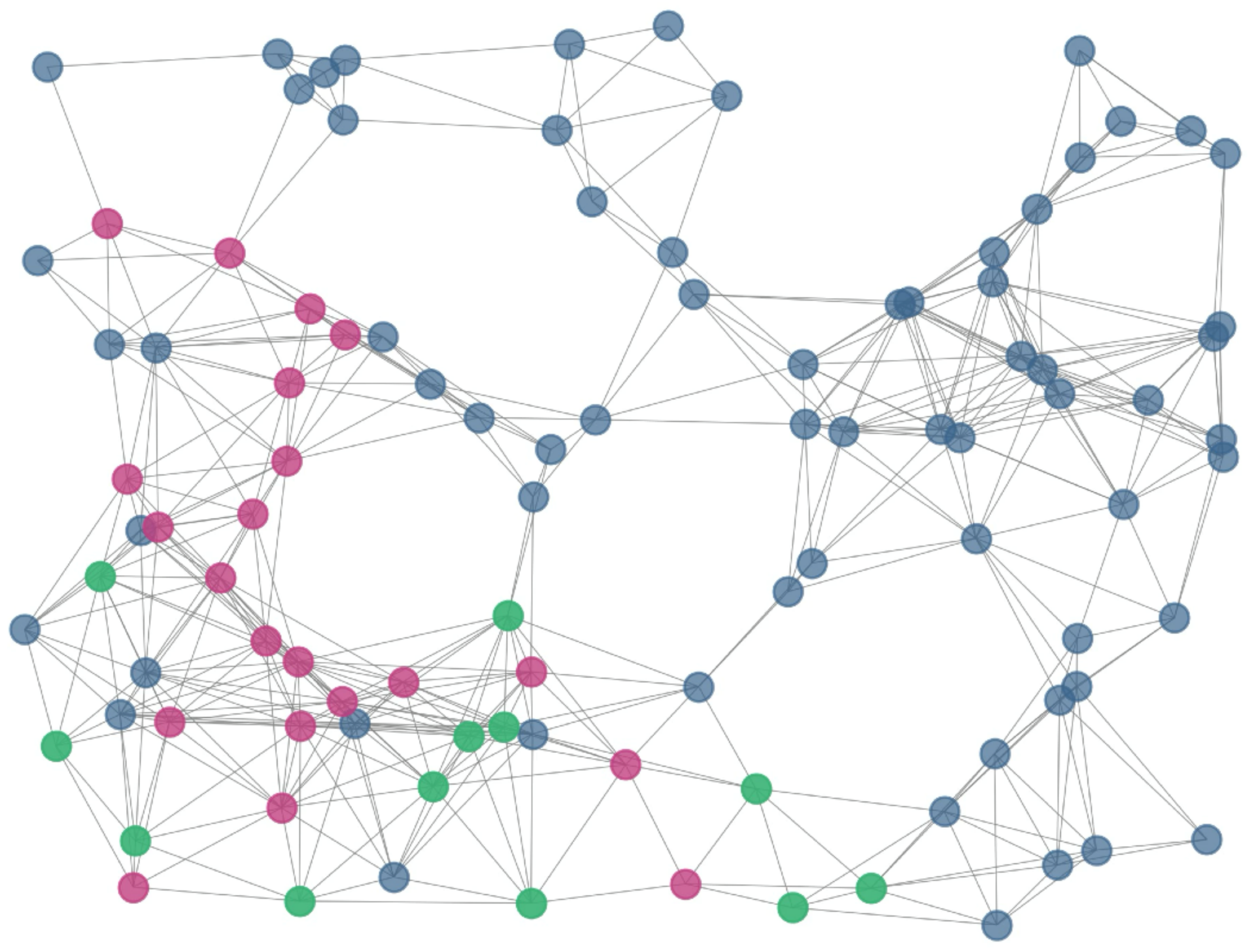
Input

- Contact graph
- SIR-type spreading model
- Nummer of vaccine doses
- Patient zero

Question

- Optimal distribution of vaccine doses?

Problem Setting



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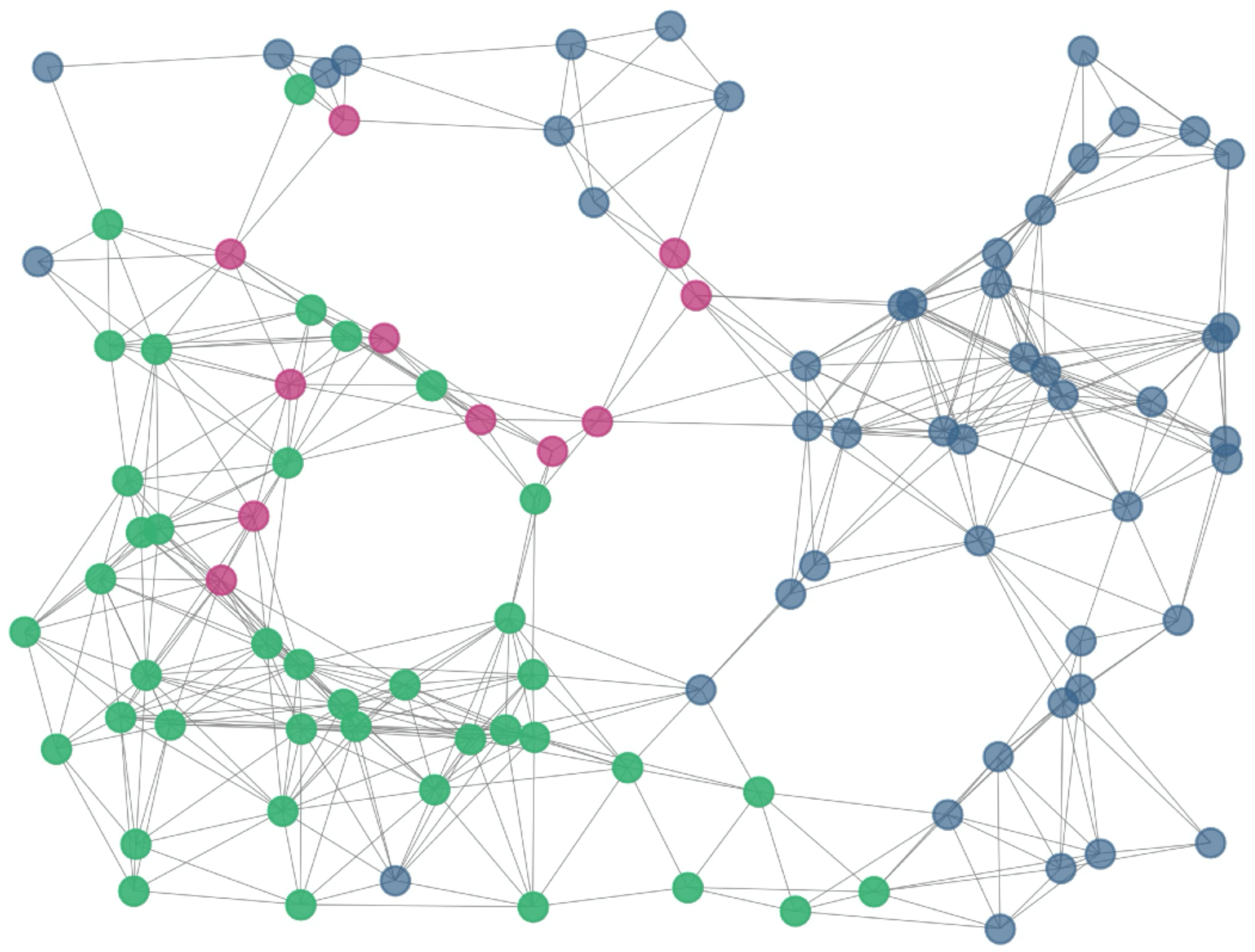
Problem Setting



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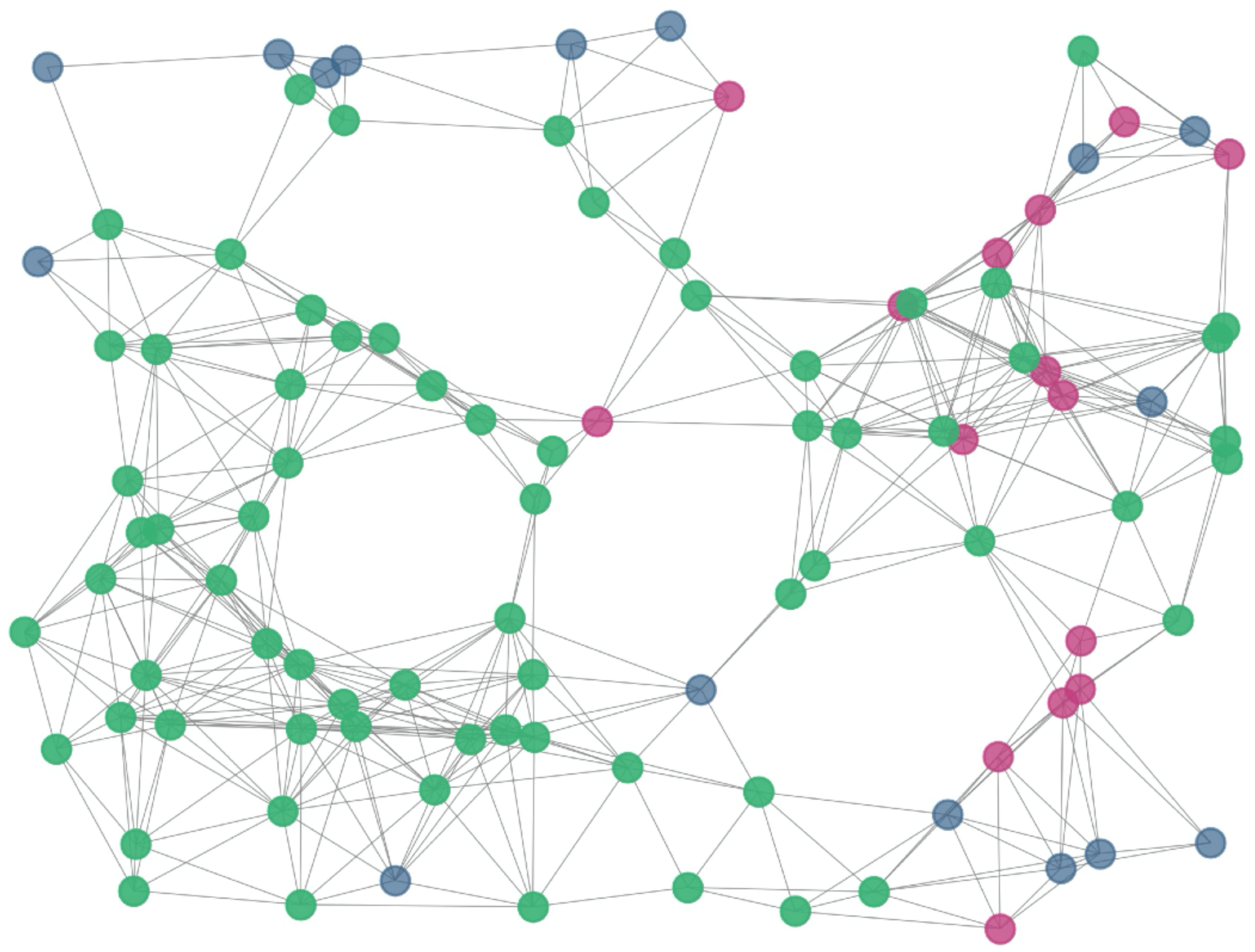

Input

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- Nummer of vaccine doses
- Patient zero

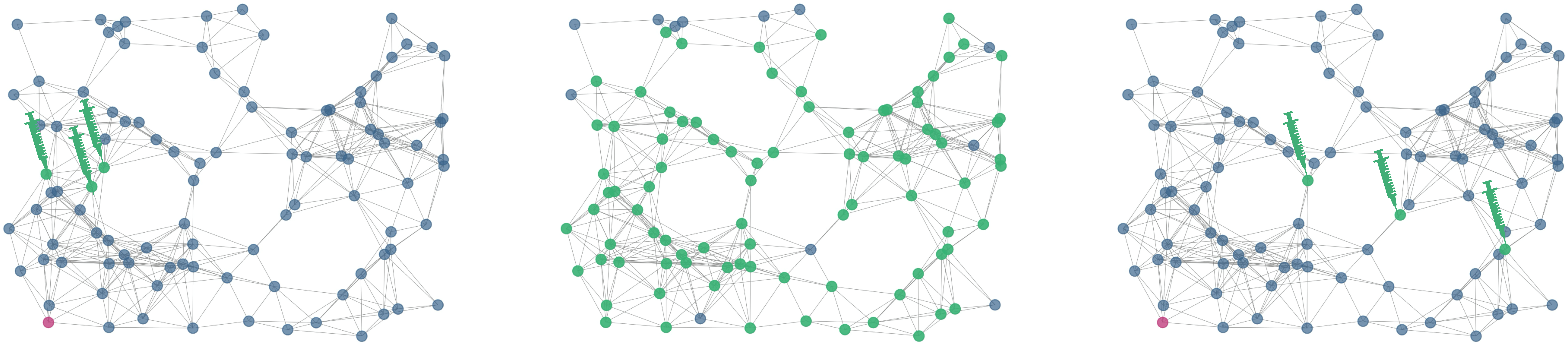
Question

- Optimal distribution of vaccine doses?

Problem Setting

Strategy 1

Strategy 2



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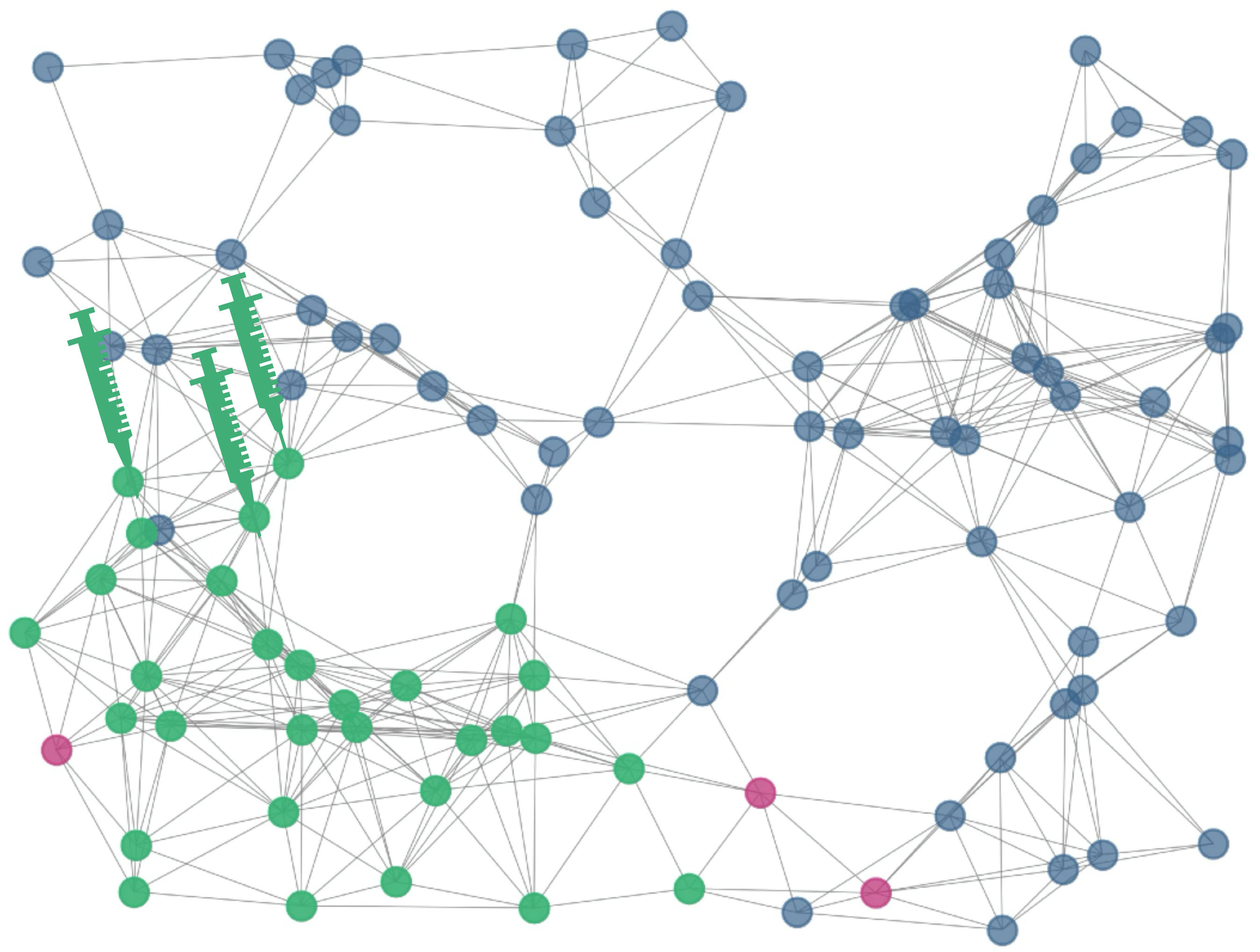
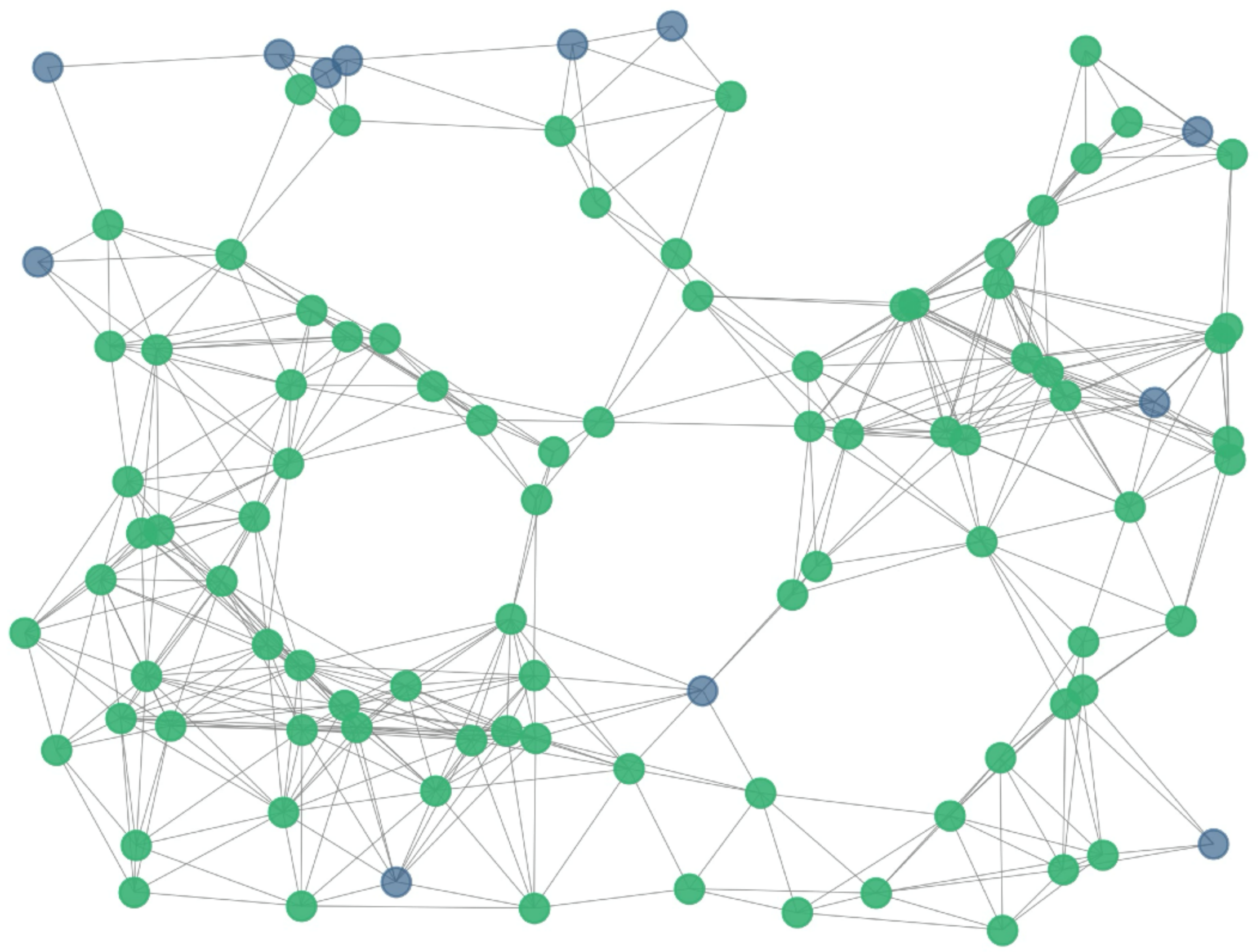
- Optimal distribution of vaccine doses?

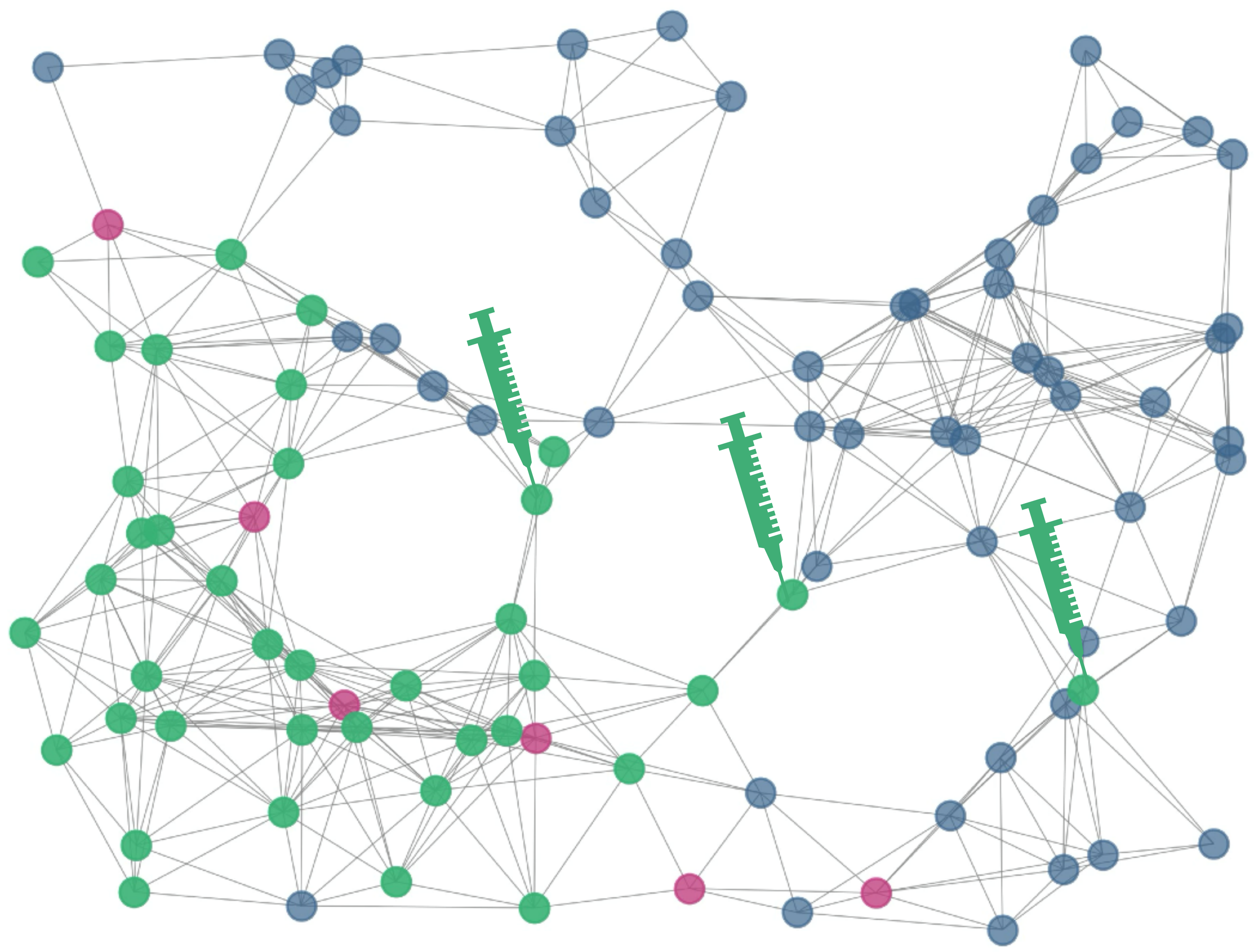
Problem Setting

Strategy 1





Strategy 2



Input

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- SIR-type spreading model
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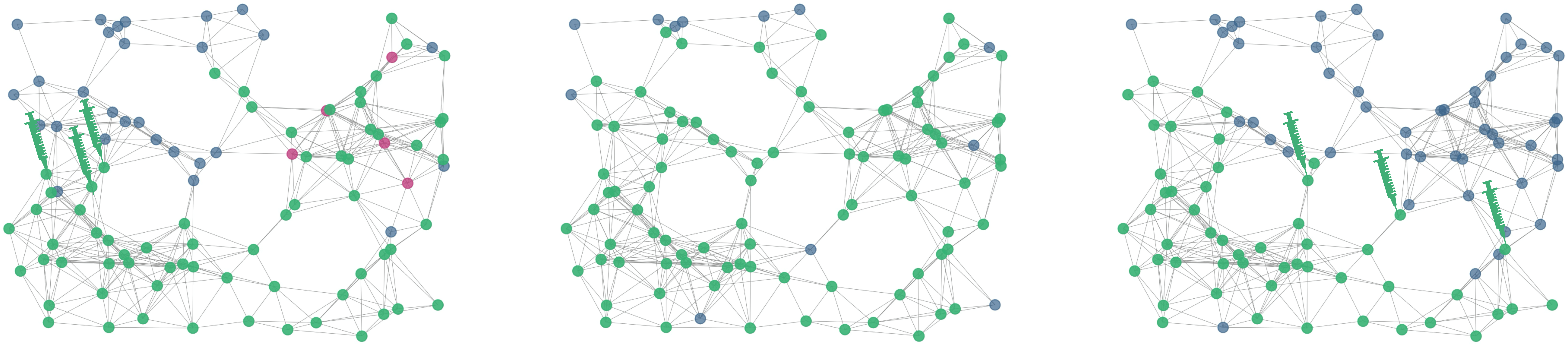
Question

- Optimal distribution of vaccine doses?

Problem Setting

Strategy 1

Strategy 2



Input

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- Nummer of vaccine doses
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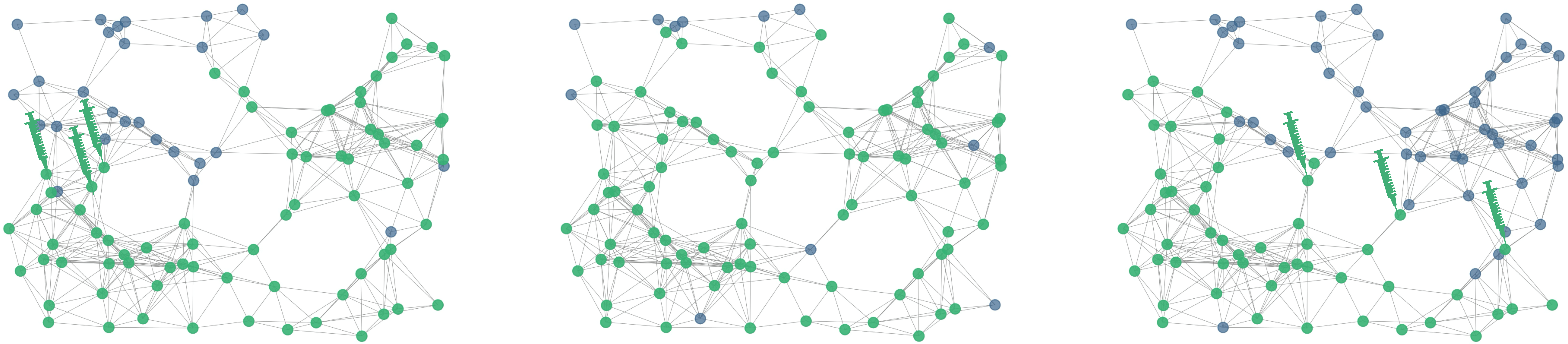
Question

- Optimal distribution of vaccine doses?

Problem Setting



Input

- Contact graph
- SIR-type spreading model
- Nummer of vaccine doses
- Patient zero

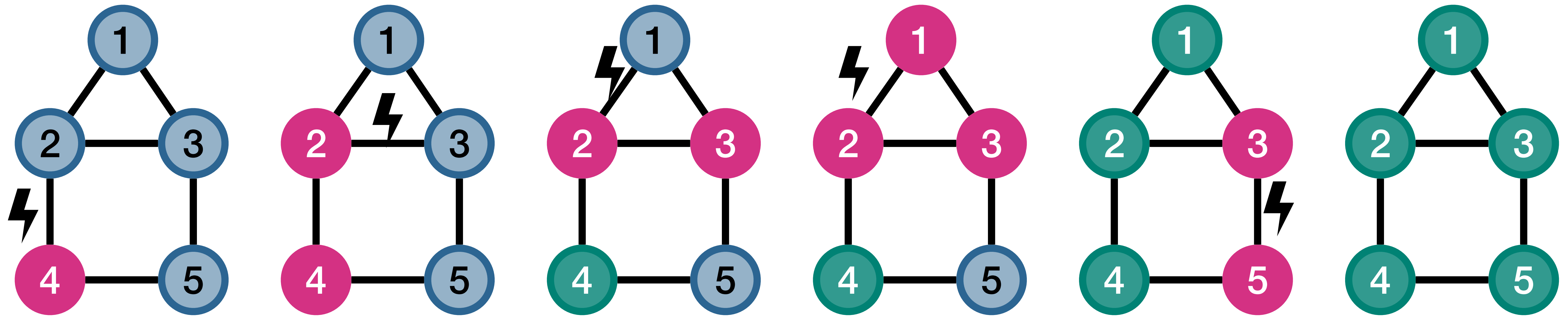
Question

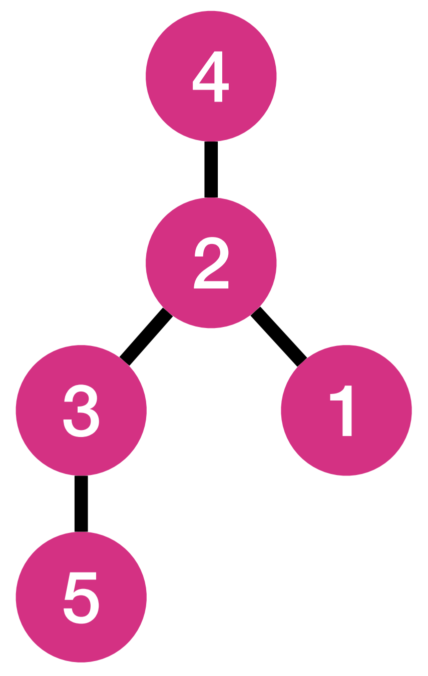
- Optimal distribution of vaccine doses?

Problem

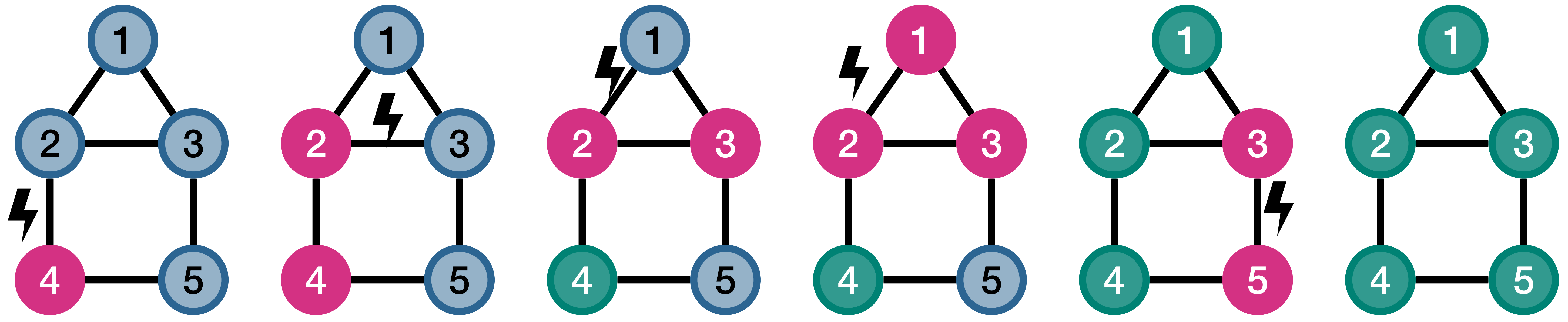
- Combinatorial explosion

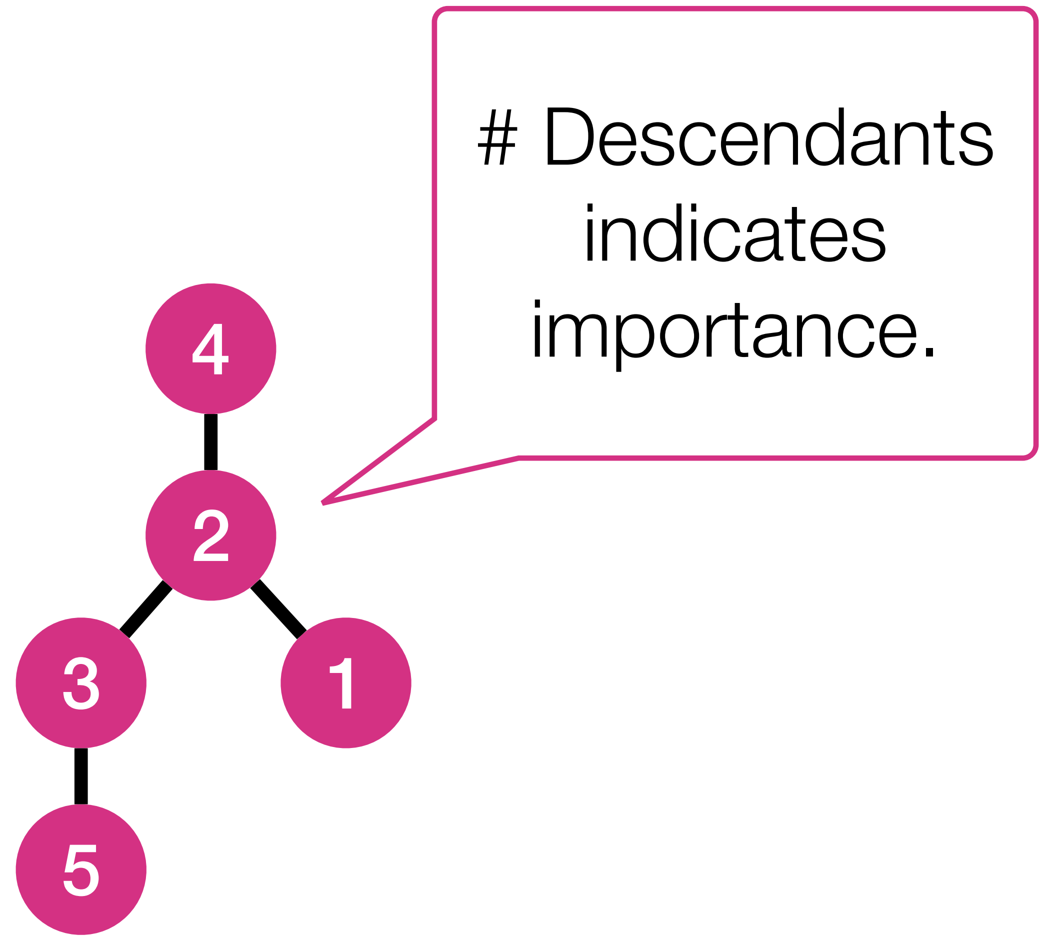
Transmission Trees



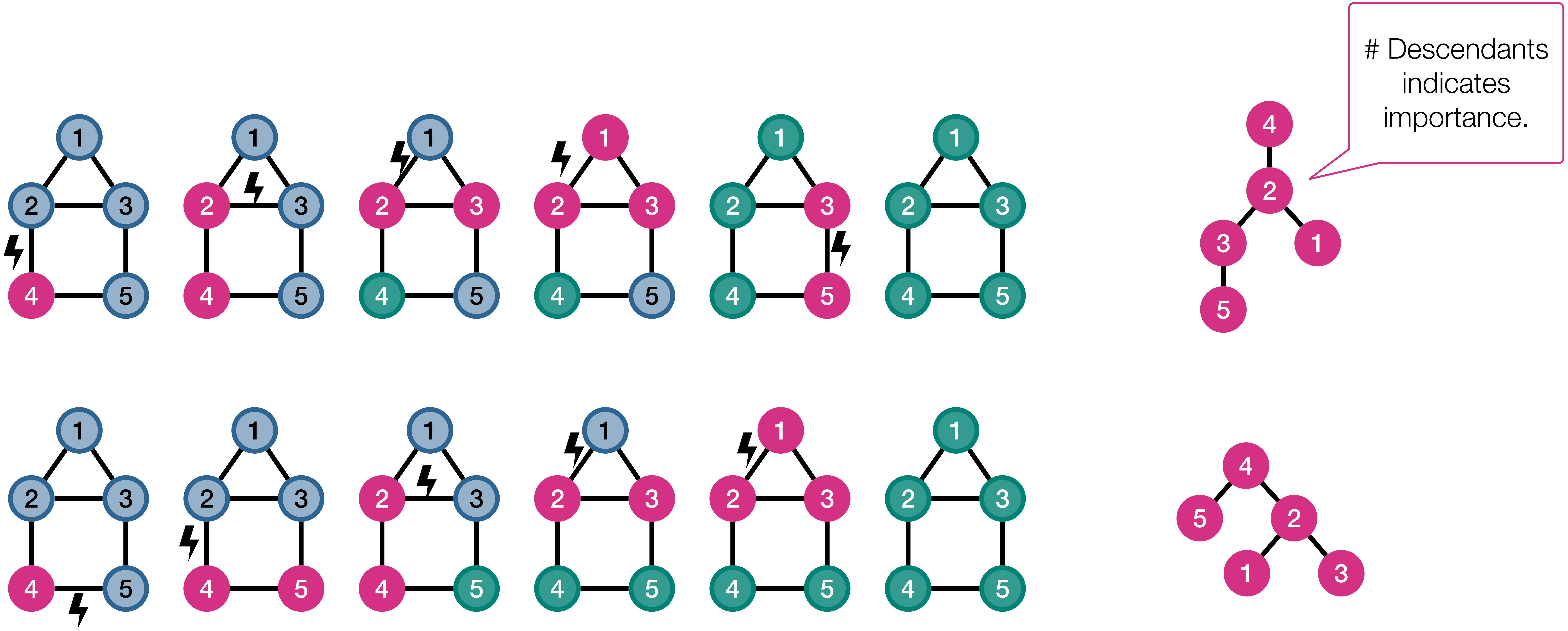


Transmission Trees



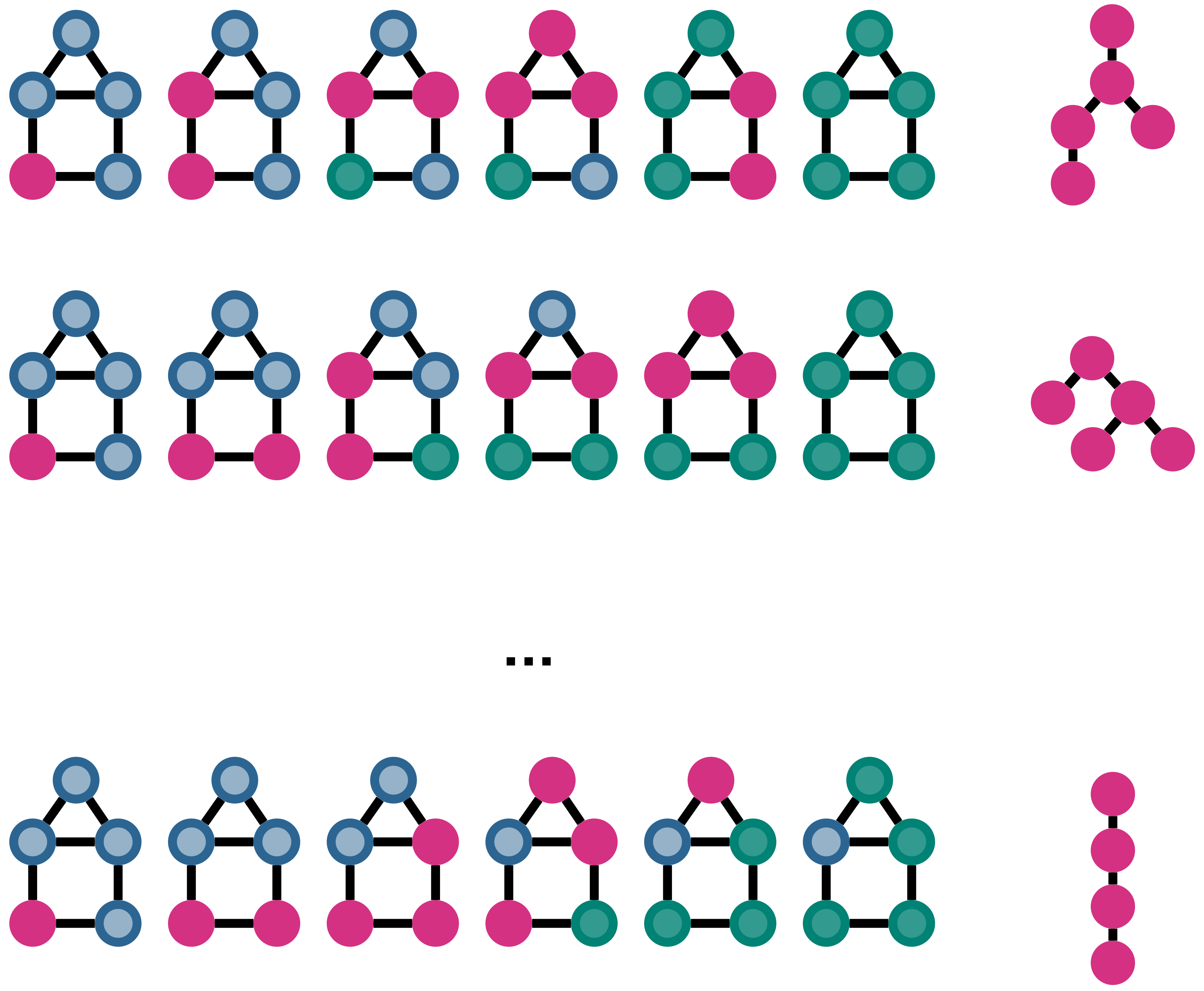


Transmission Trees

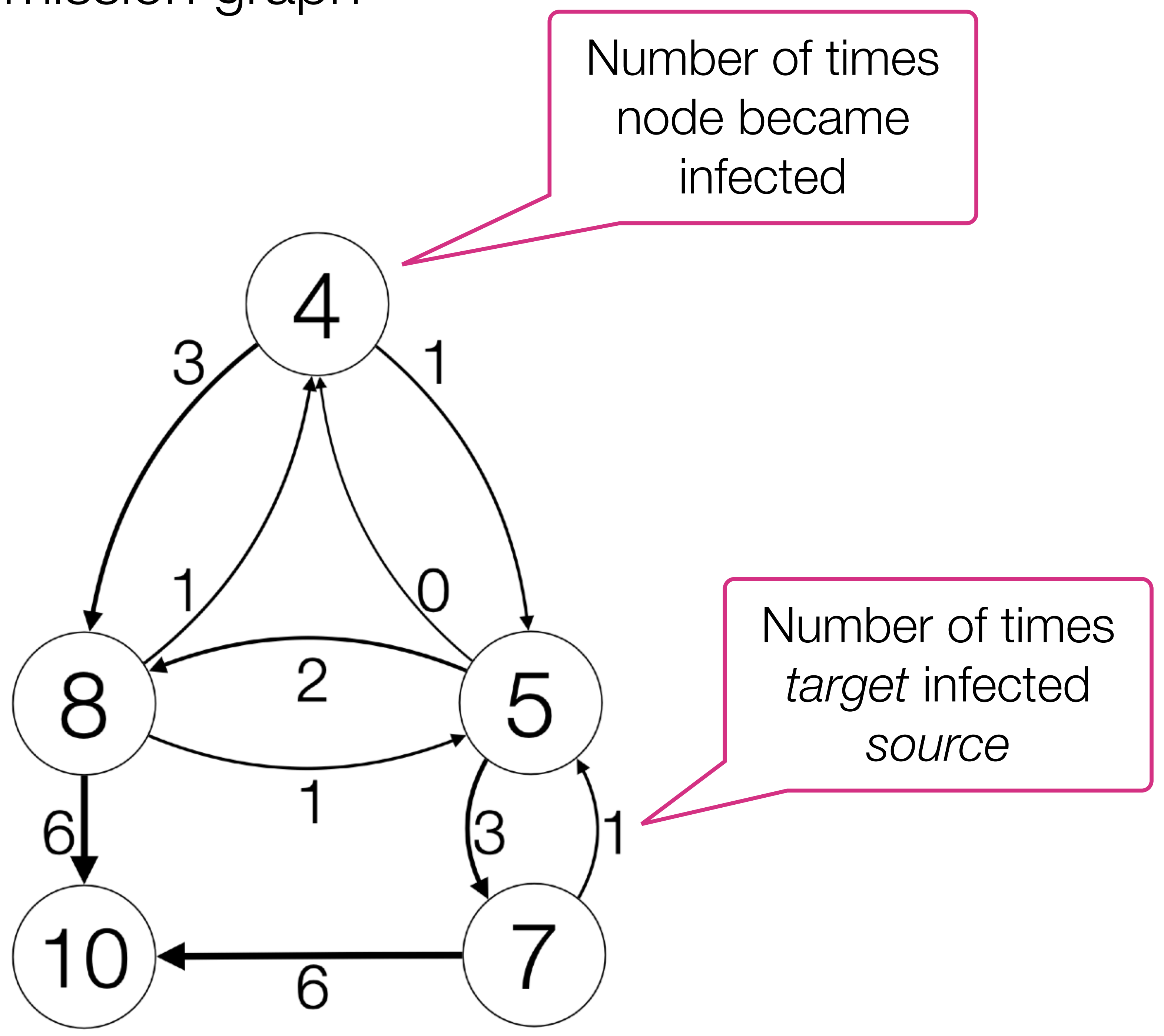


From Trees to Graphs

Simulation runs
(10 samples)

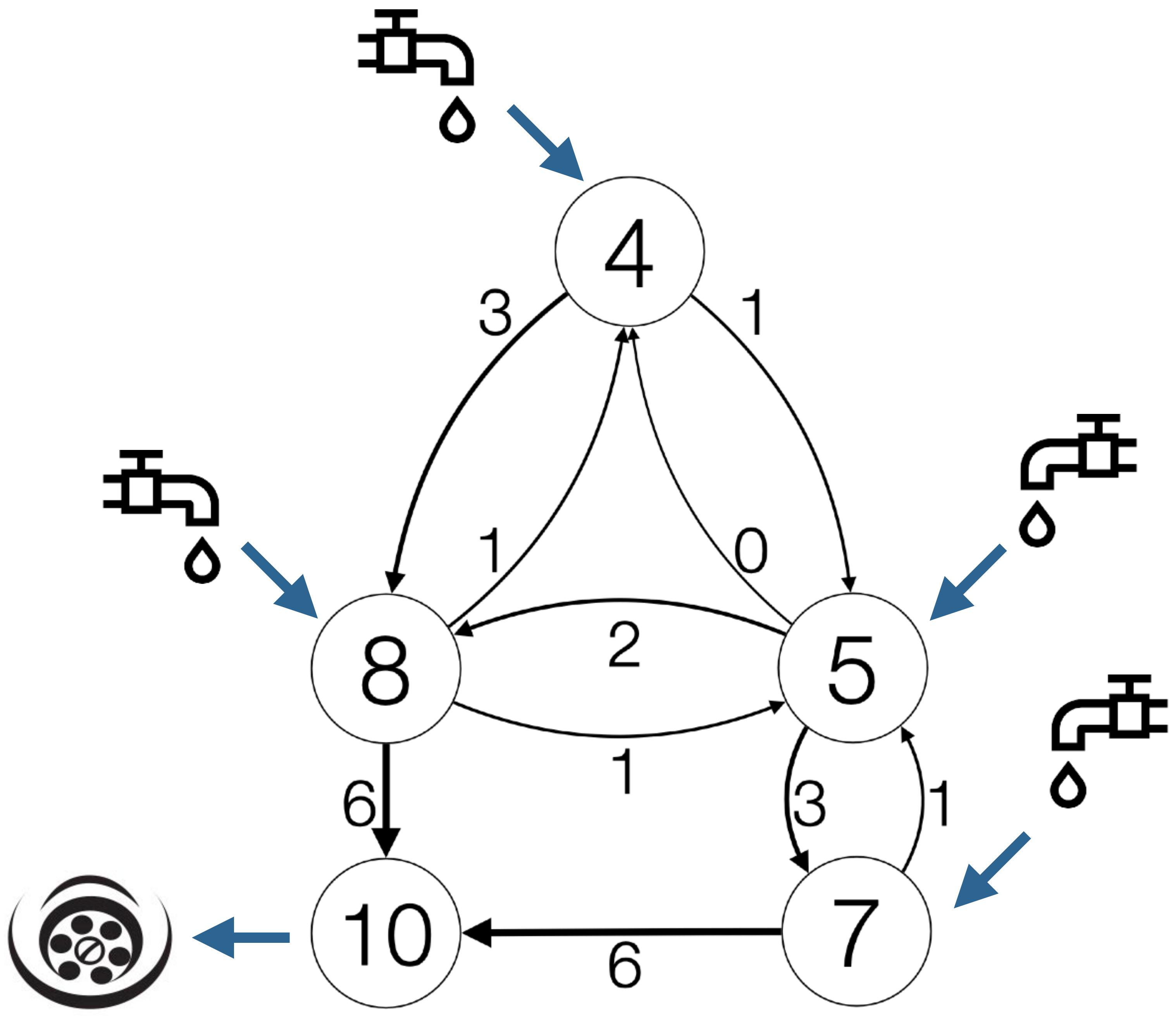


Transmission graph



Flow Analysis

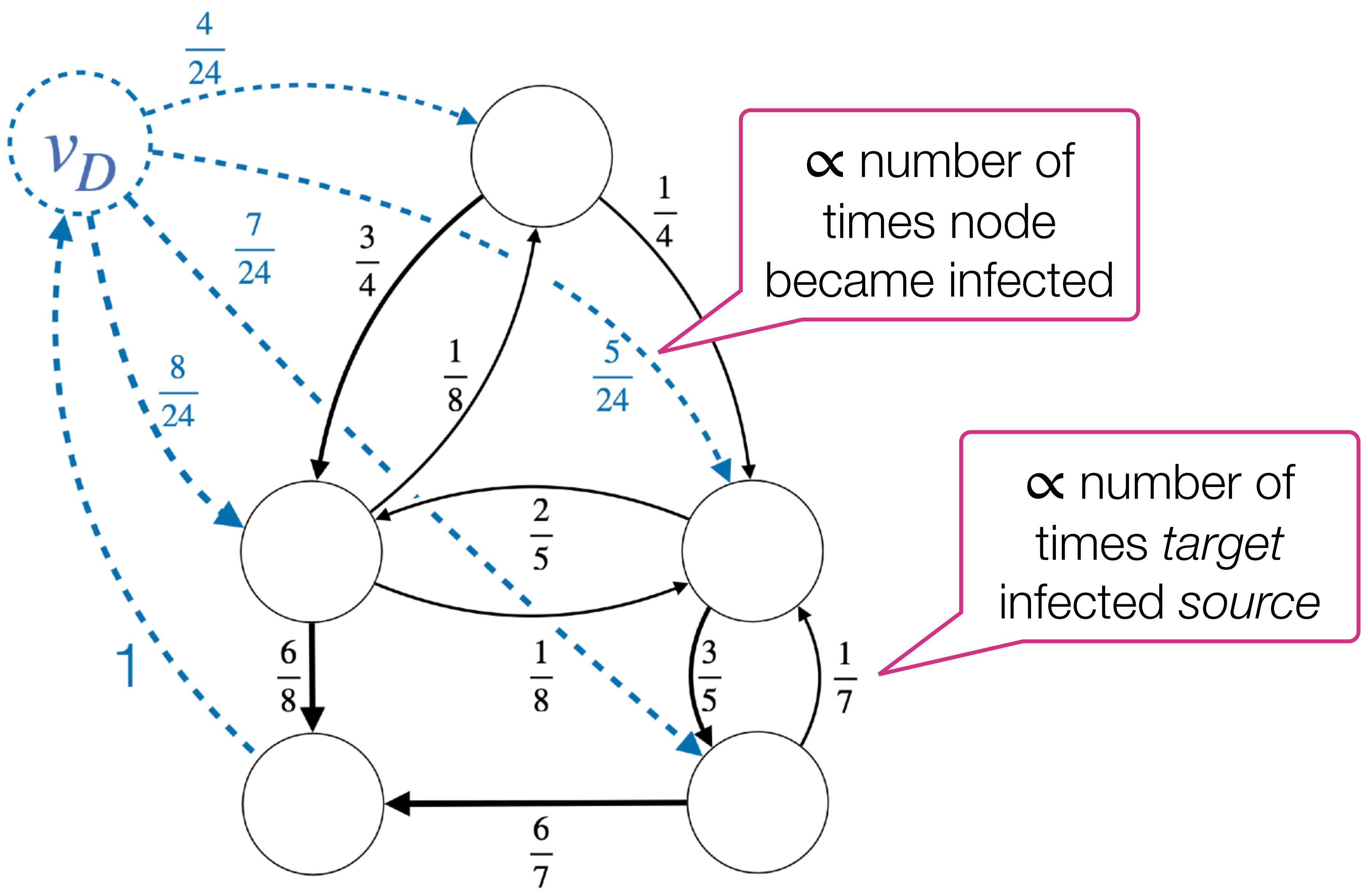
Transmission graph



- **Source**: Each infected node
- **Sink**: Patient zero
- Reversed direction of propagation
- Flow strength = proportional to transmission impact.

Flows as Random Walks

Transmission graph



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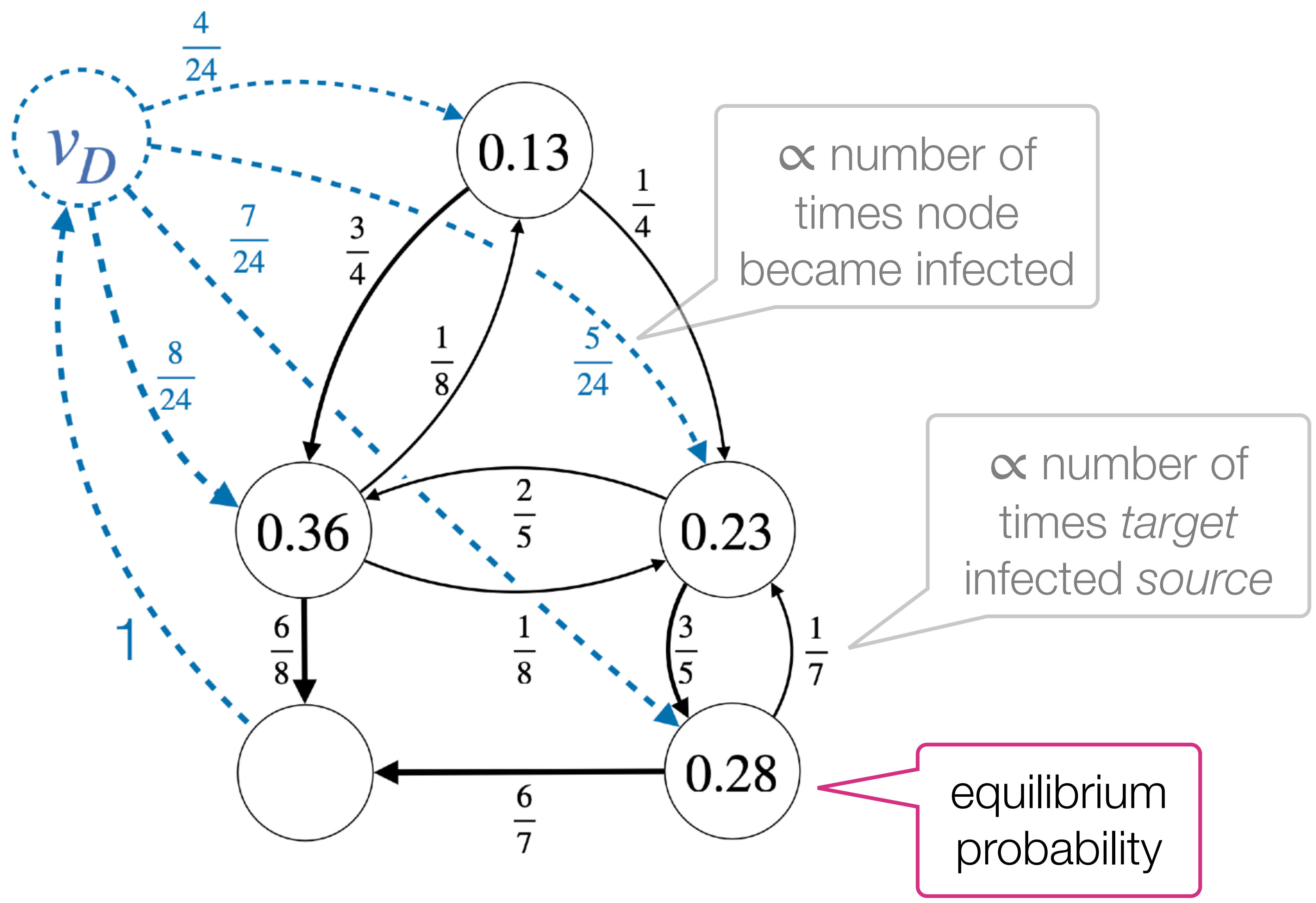
Flows as Random Walks

Transmission graph



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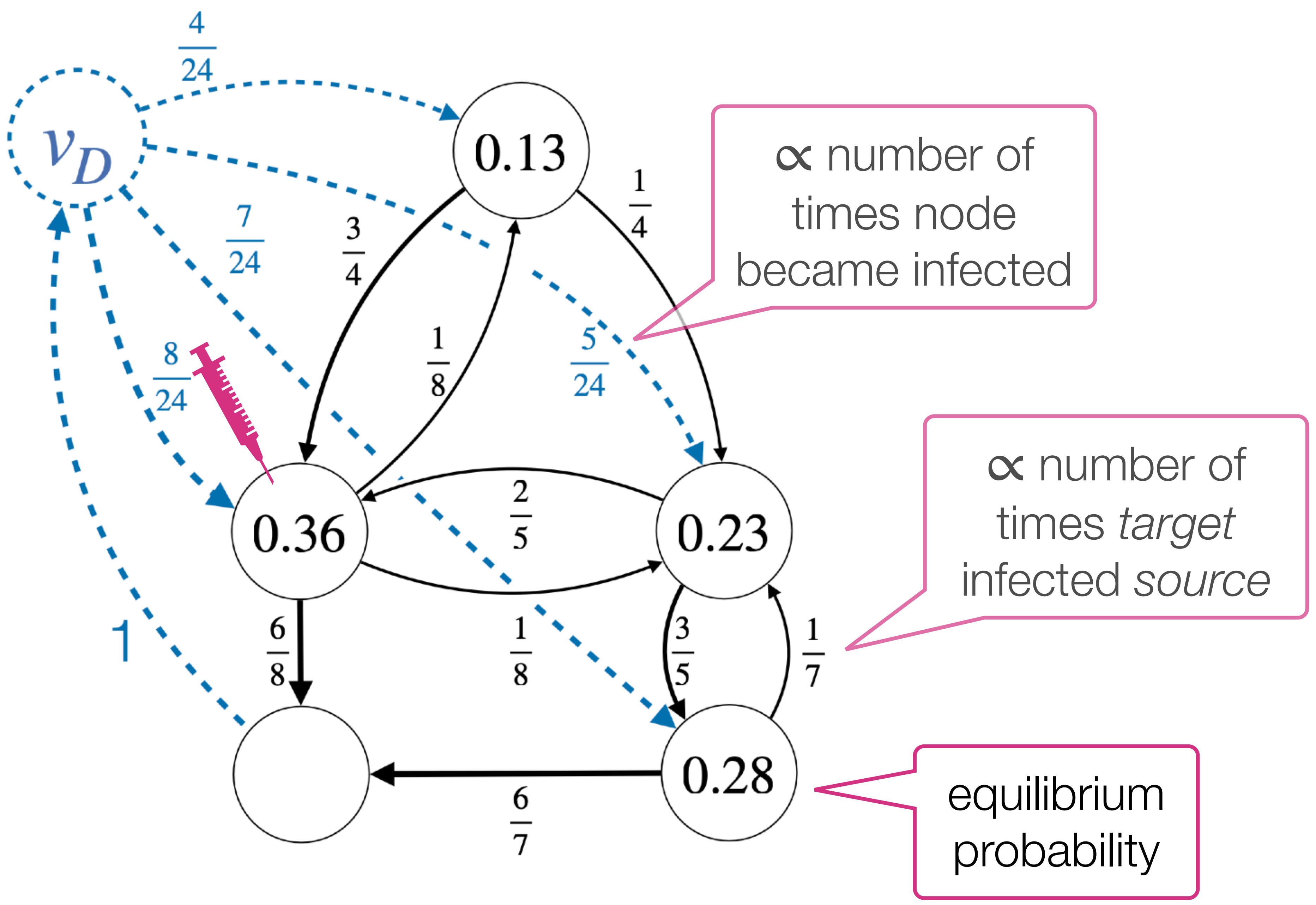
Flows as Random Walks

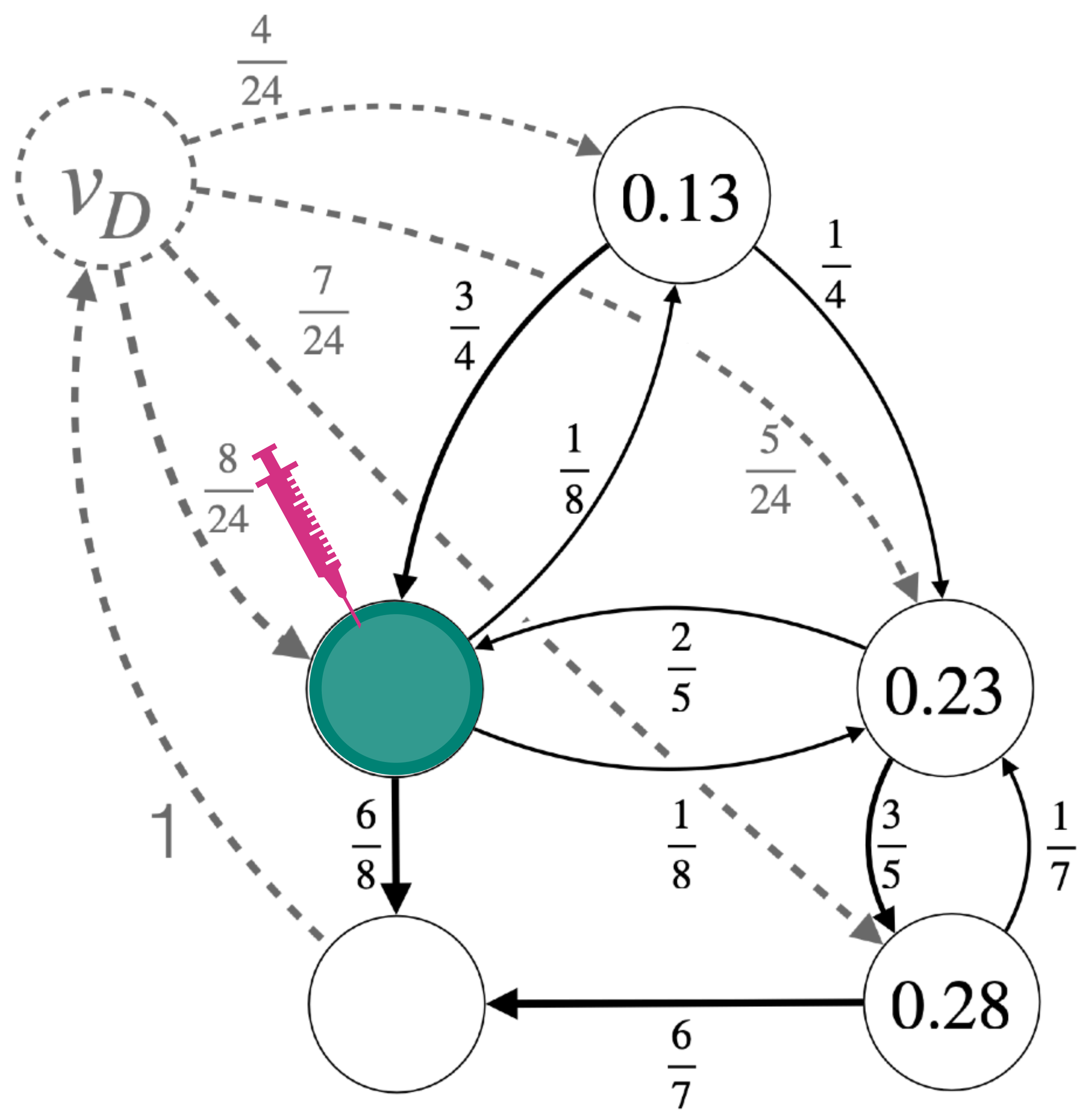
Transmission graph



- **Source**: Each infected node
- **Sink**: Patient zero
- Reversed direction of propagation
- Flow strength = proportional to transmission impact.

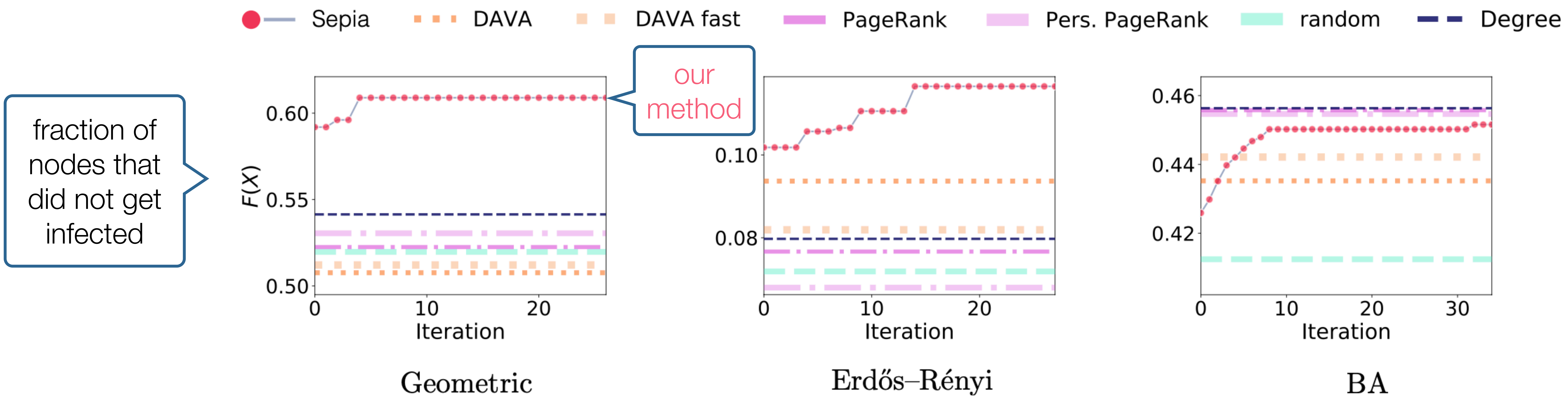
Optimization

Transmission graph



Vaccination
+
Recompute impact score
+
Iterative optimization

Control: Results



(higher is better)

Agenda

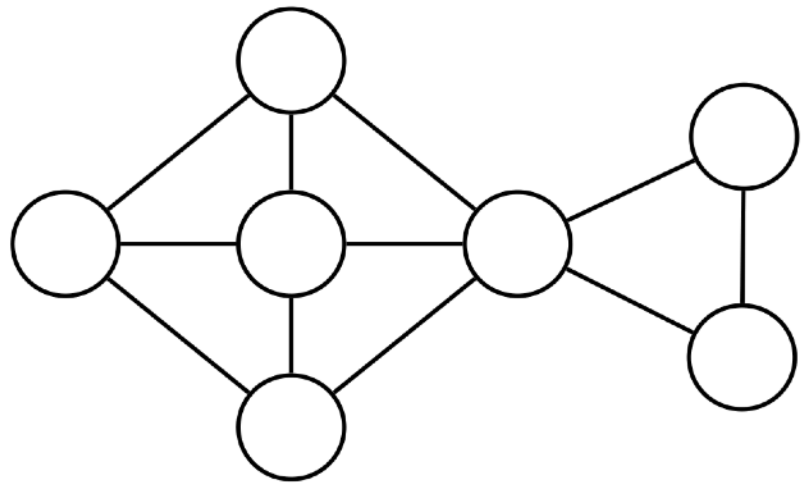
METHODS

COVID
(NON-)MARKOVIAN SIMULATION
CONTROL
INFERENCE

Pipeline

Inference

Probing



?

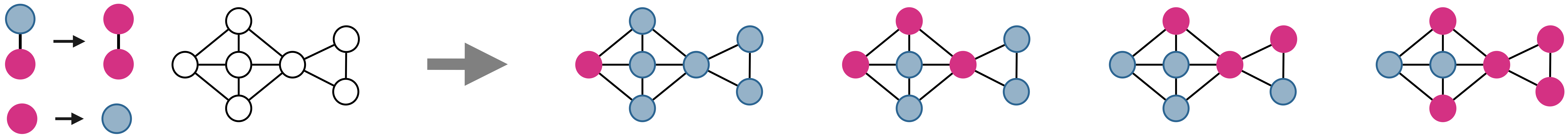
- Expected number infected individuals?
- Final epidemic size?
- Worst case number of casualties?
- Reduce the number of infections?

Observations

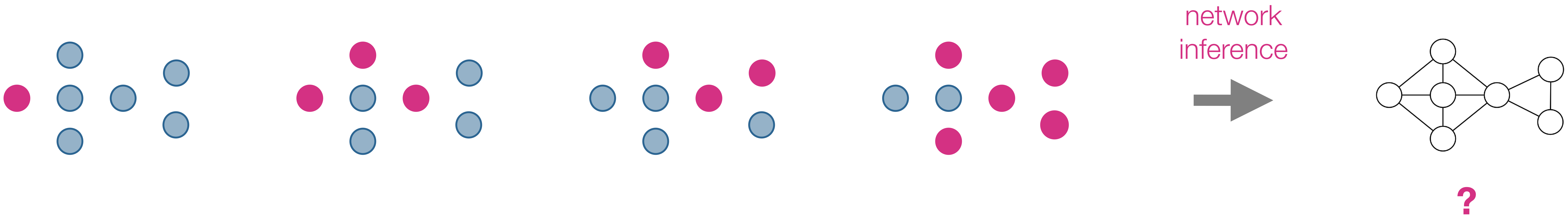
Questions

Problem Setting

Generation:

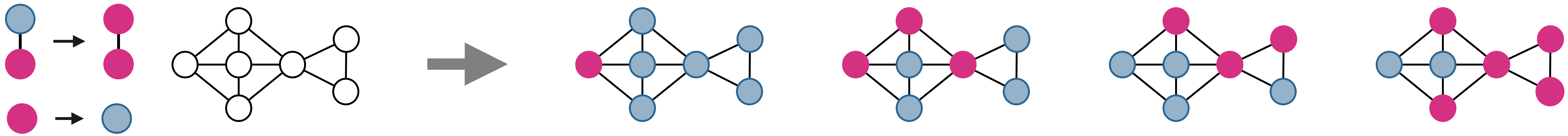


Our task:



Problem Setting

Generation:



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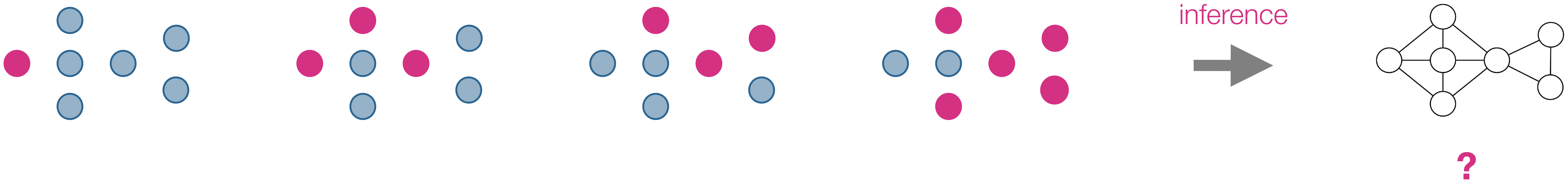
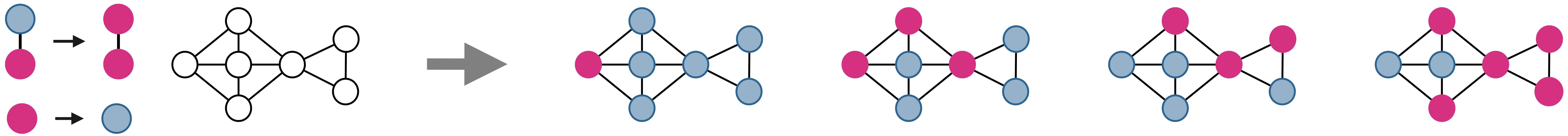


- Node-wise observations
- **Typically:** from time-series data
- **Here:** from independent snapshots

Problem Setting

Generation:



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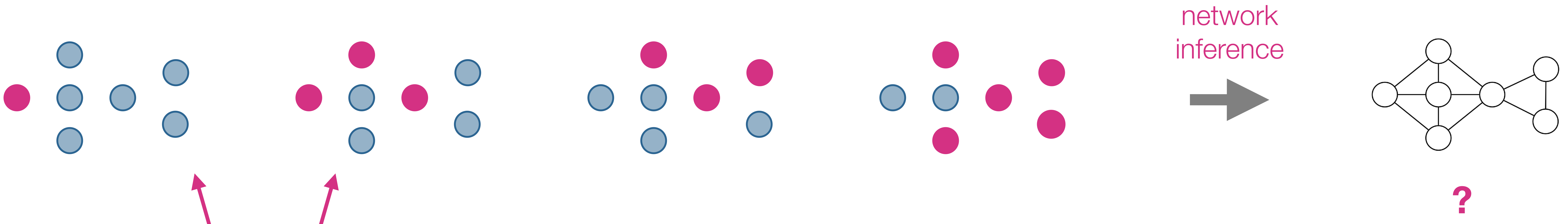


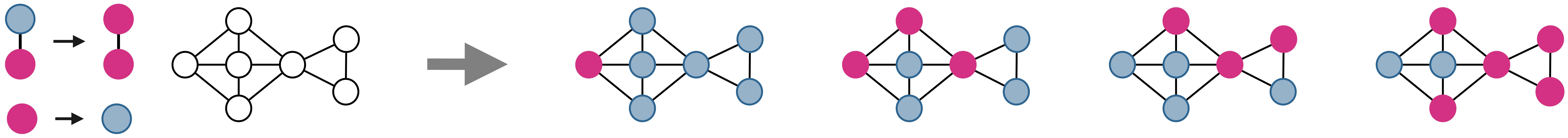
Do not assume any correlation.

- Node-wise observations
- **Typically:** from time-series data
- **Here:** from independent snapshots

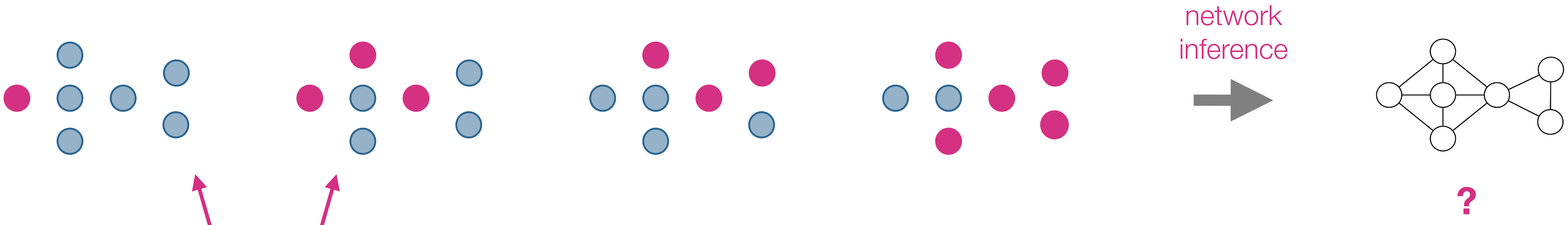
Problem Setting

Unknown dynamical model.

Generation:



Our task:



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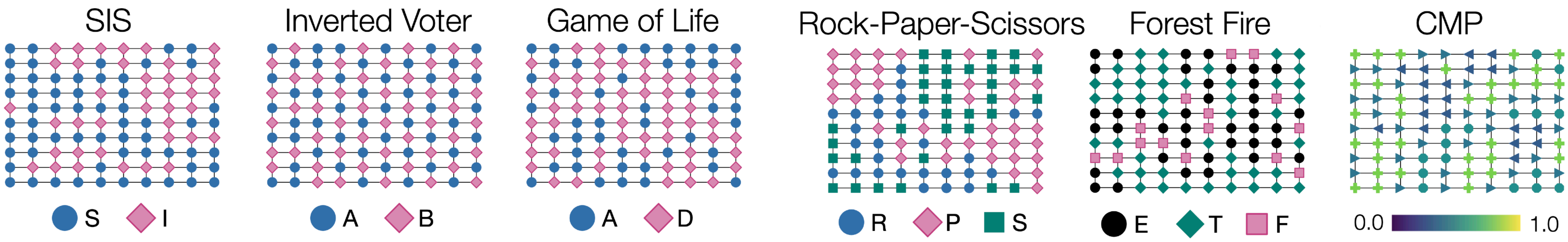
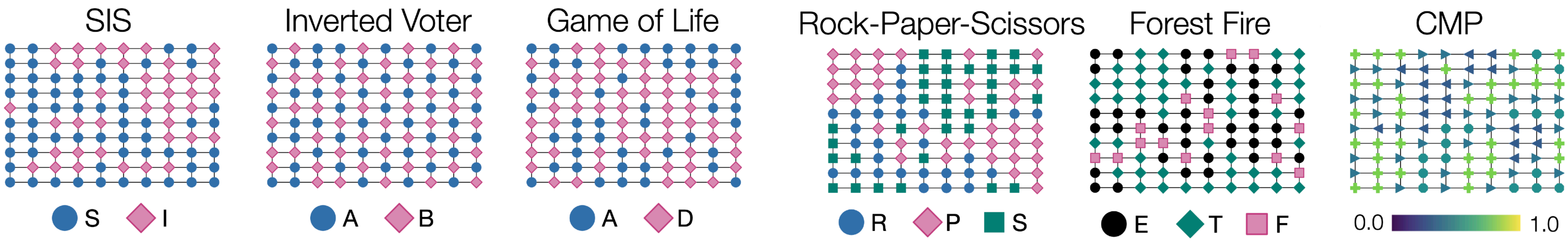
Snapshots



- **Given**: Set of independent snapshots
- **Unknown**: Interaction graph and dynamical laws
- **Task**: Find interaction graph “*best fitting*” the observed data
- **Assumption**: Patterns result from local interactions

Snapshots



- **Given**: Set of independent snapshots
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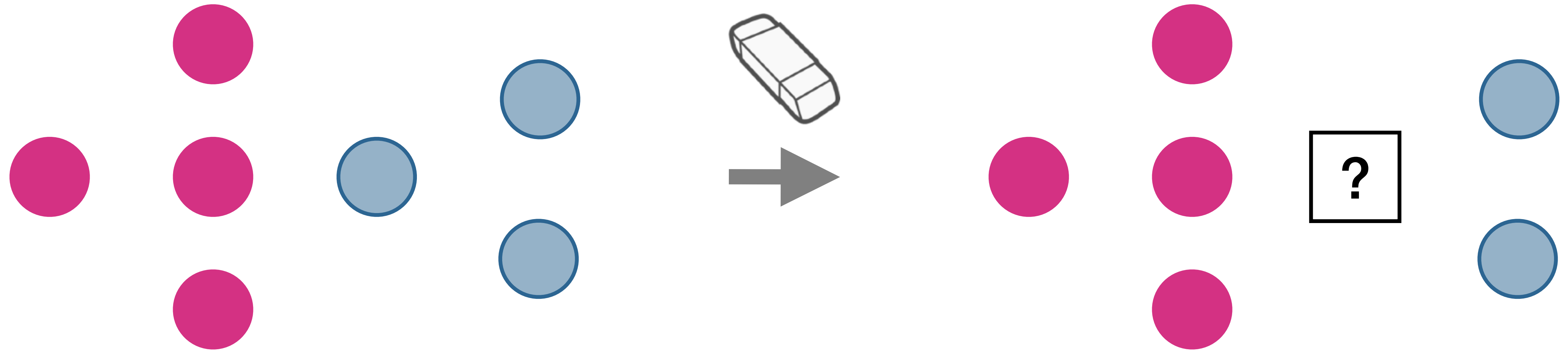
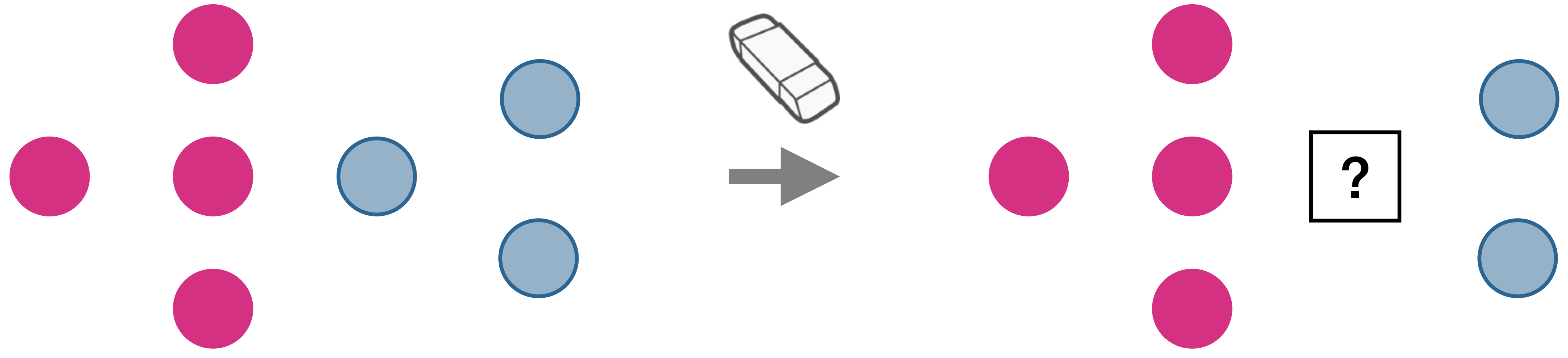
Idea

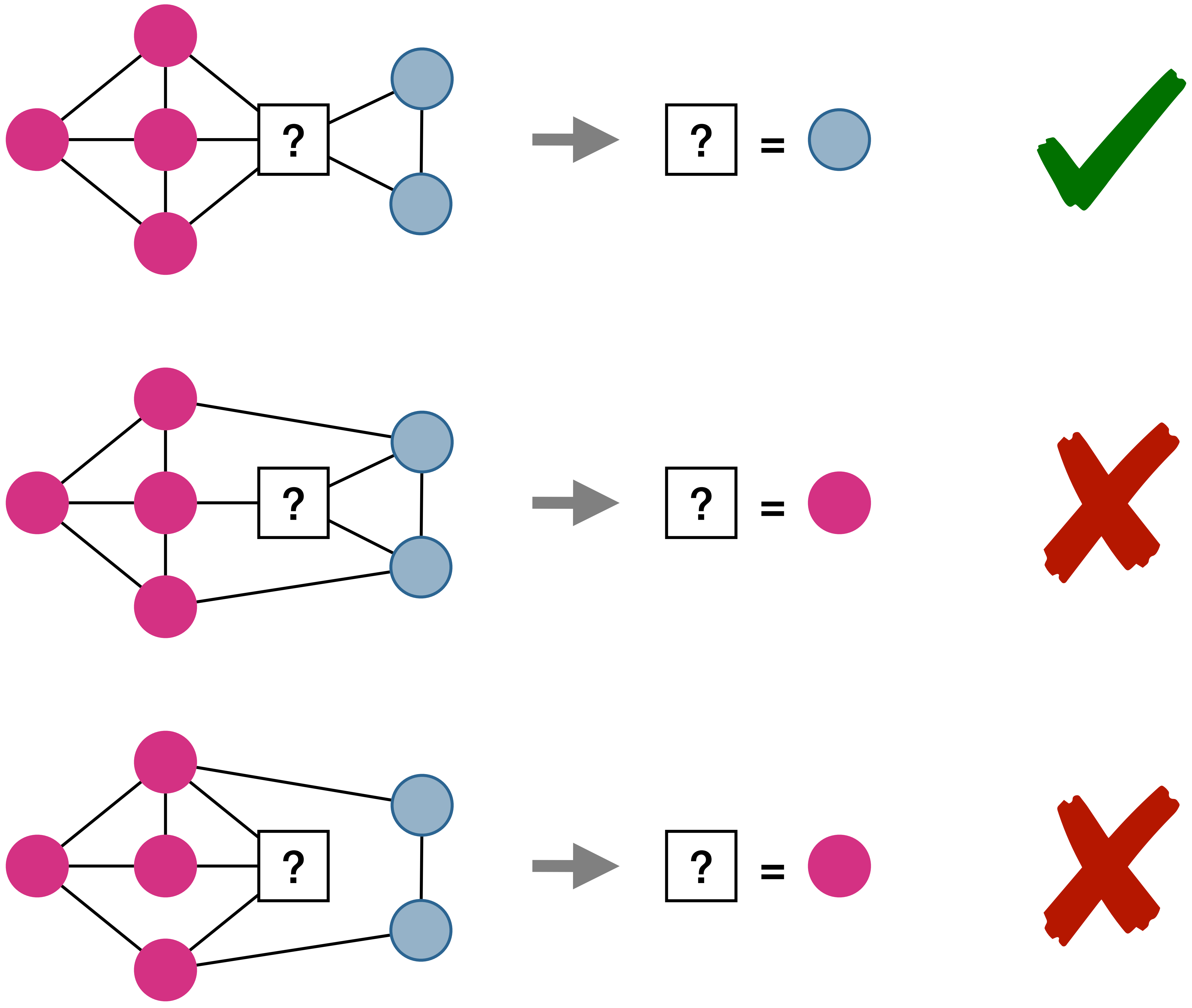


Hypothesis:

The ground truth graph allows to predict a node's states from its neighborhood with the highest accuracy.

Idea





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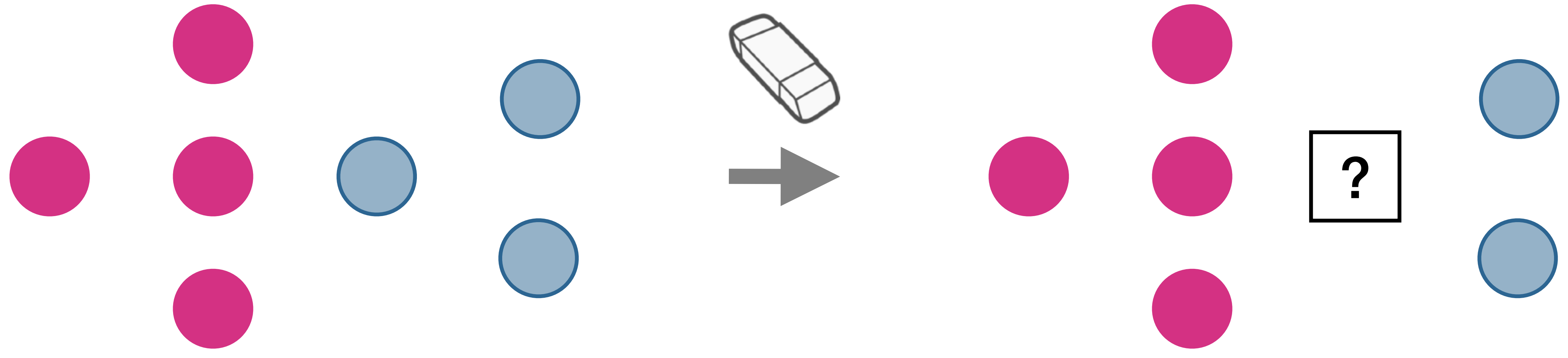
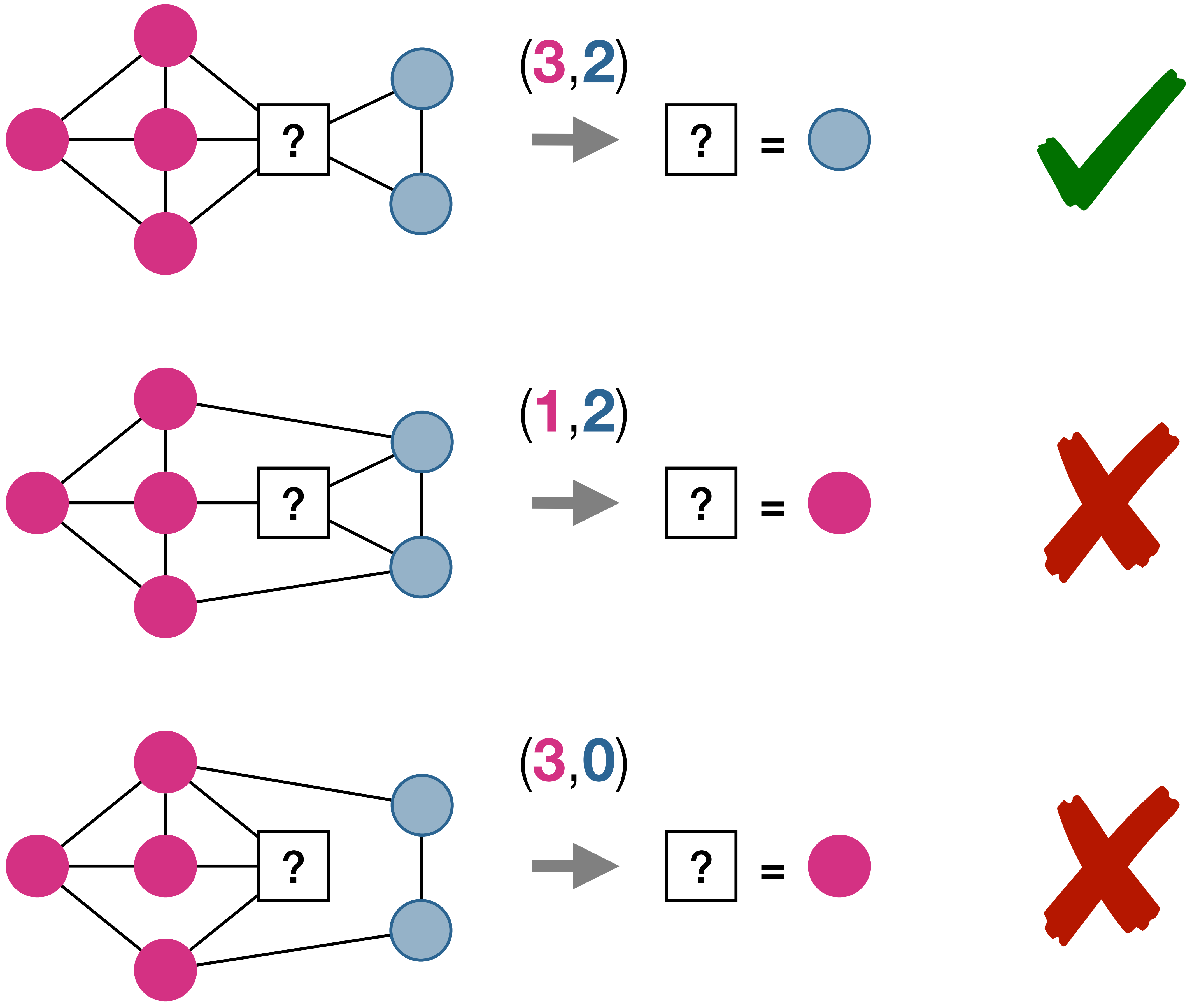


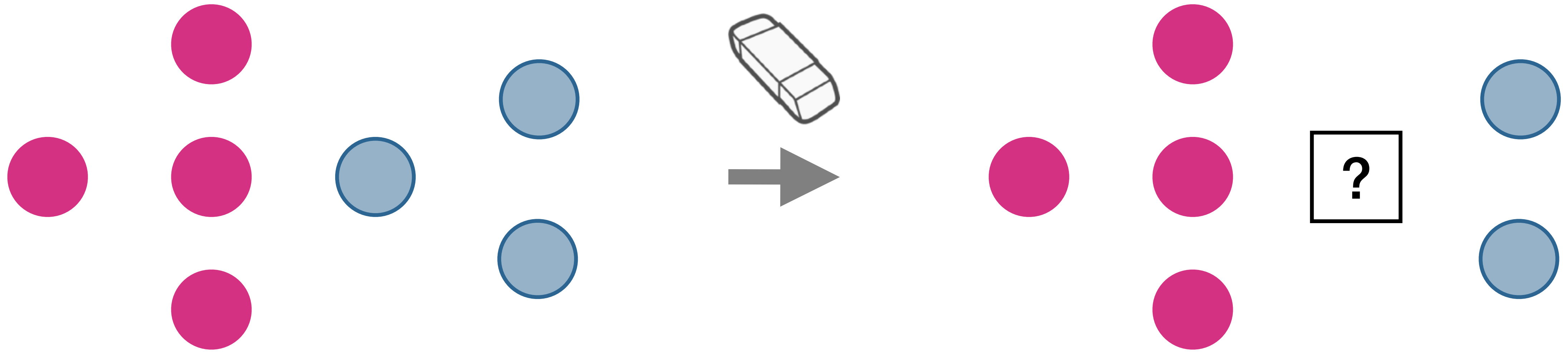


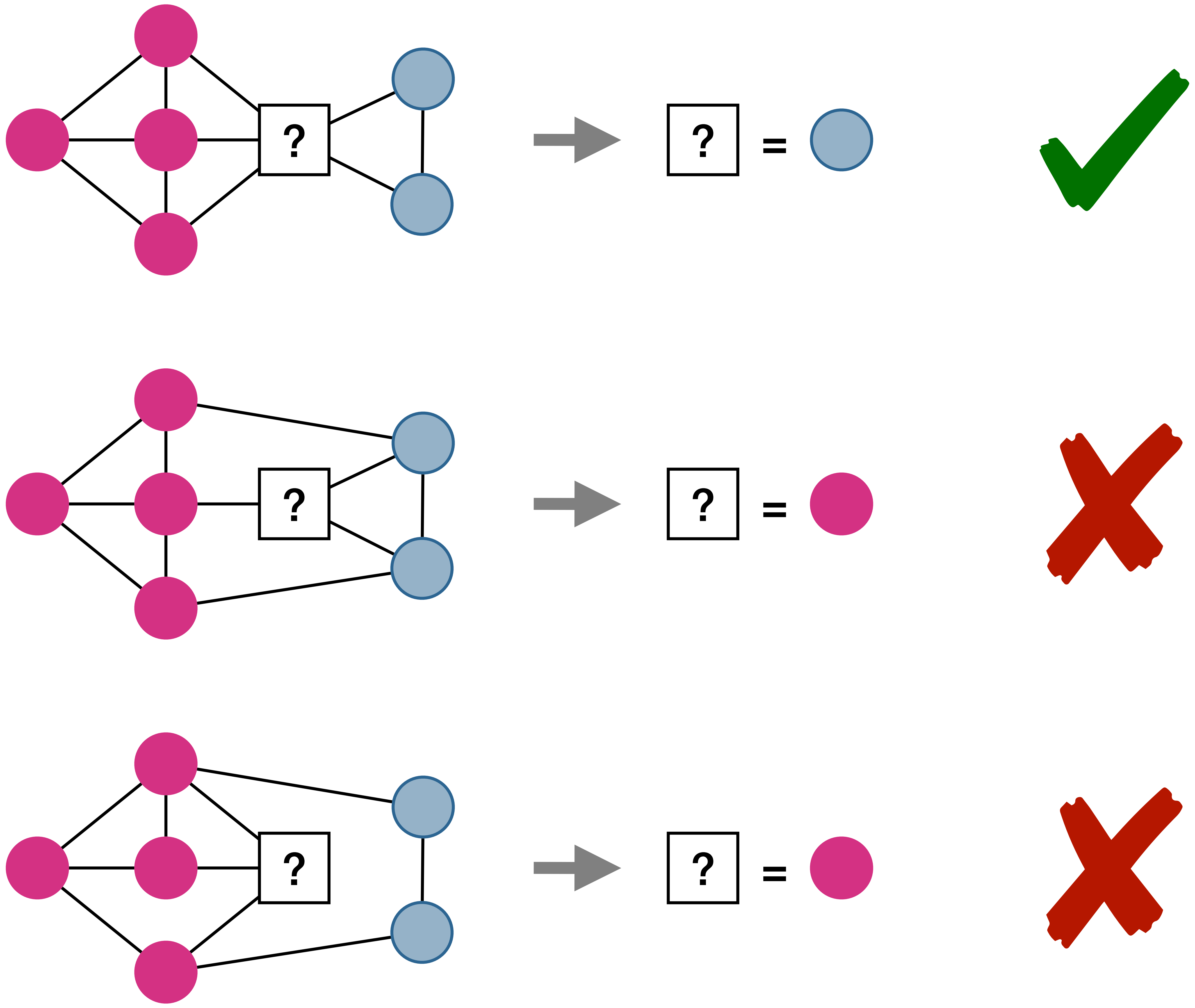
Hypothesis:

The ground truth graph allows to predict a node's states from its neighborhood with the highest accuracy.

Idea

Problem: search space size





Hypothesis:

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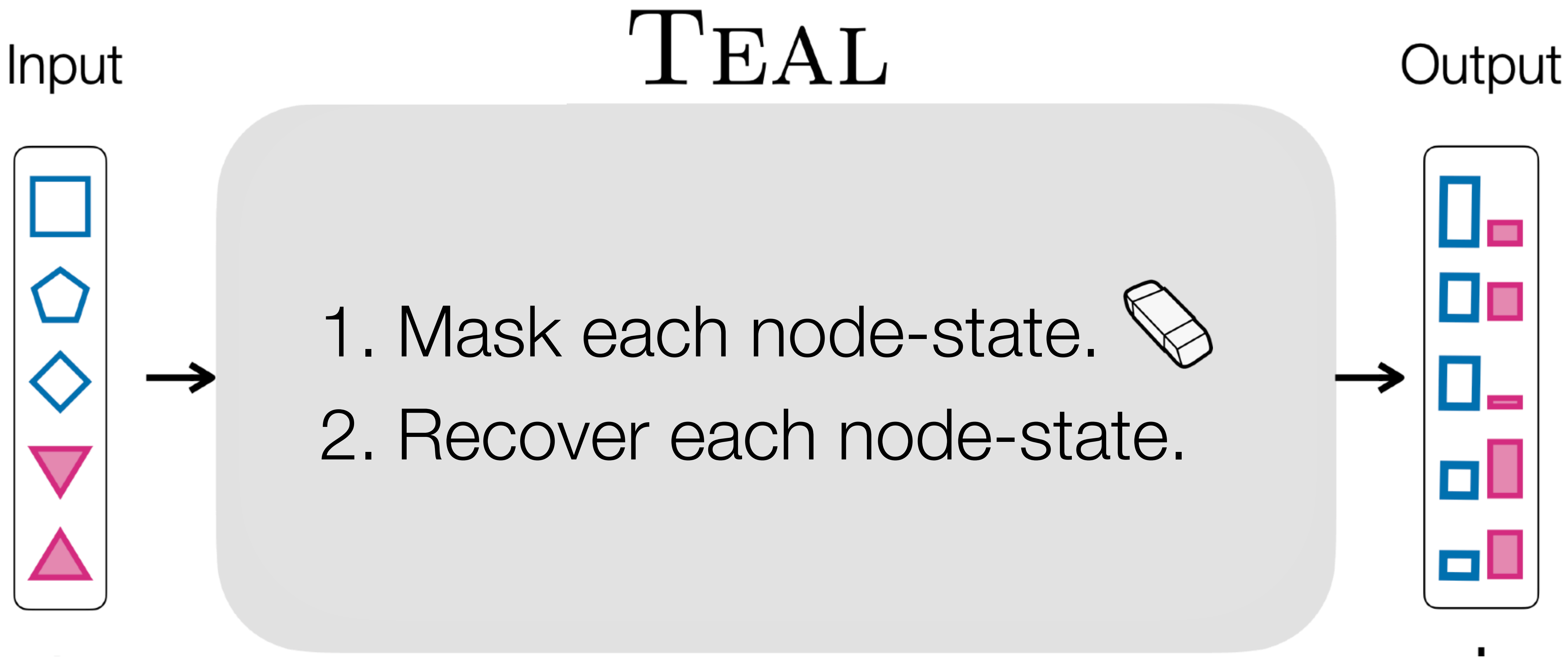
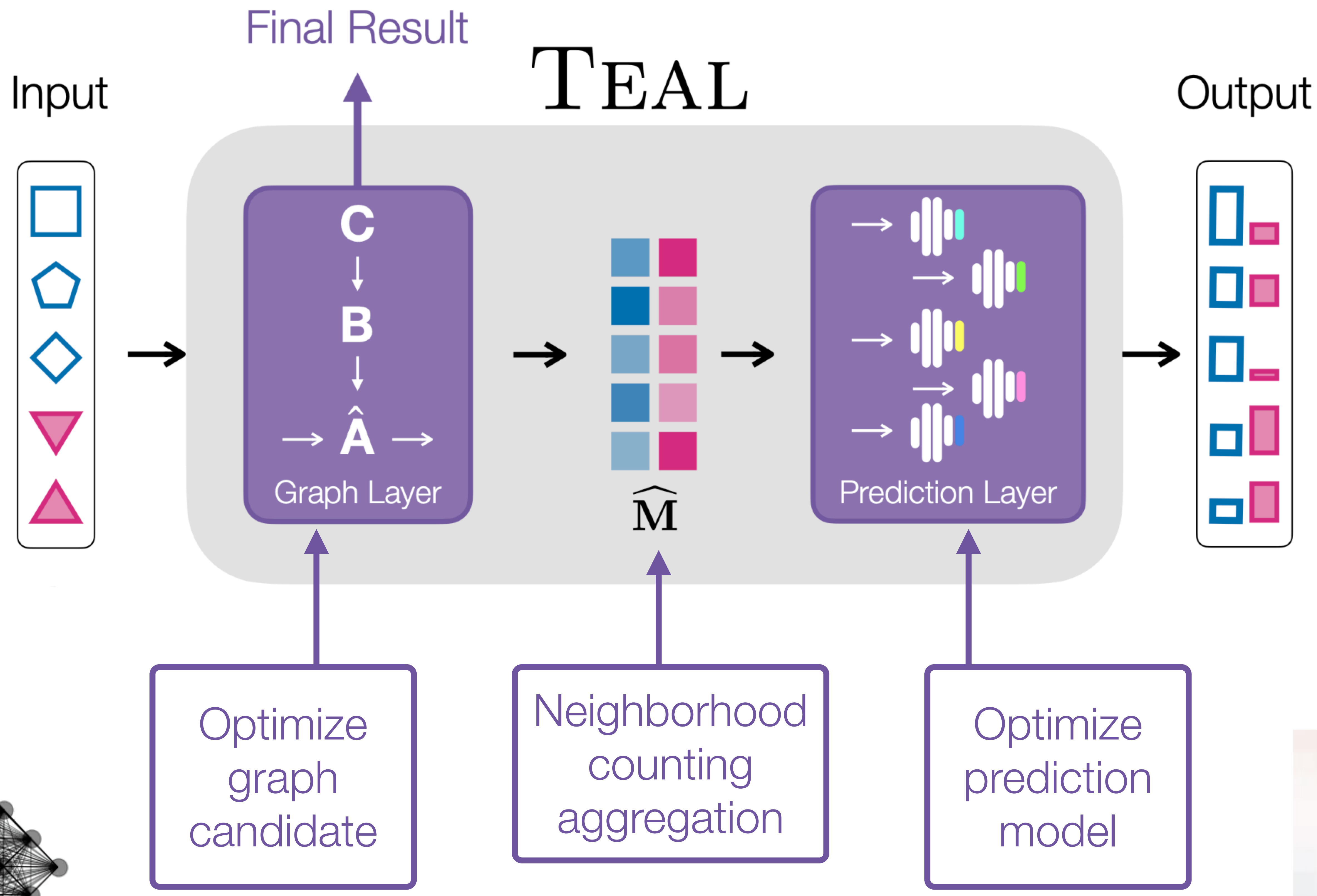
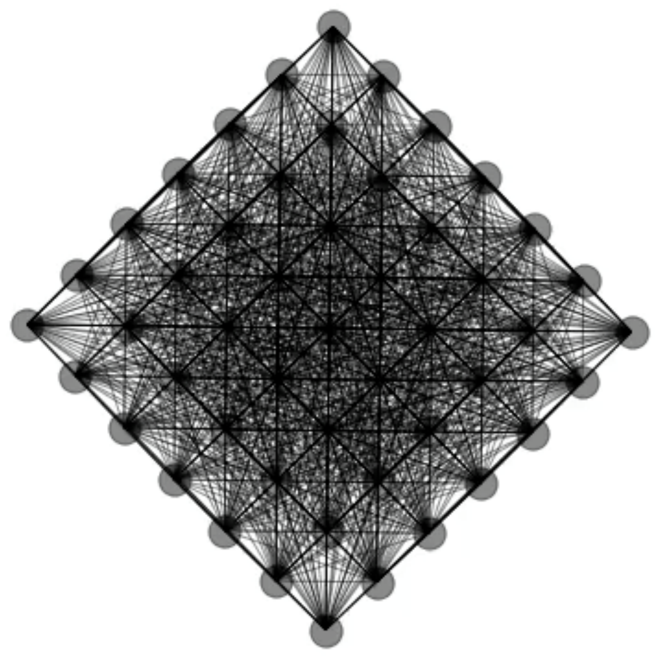
Our Method

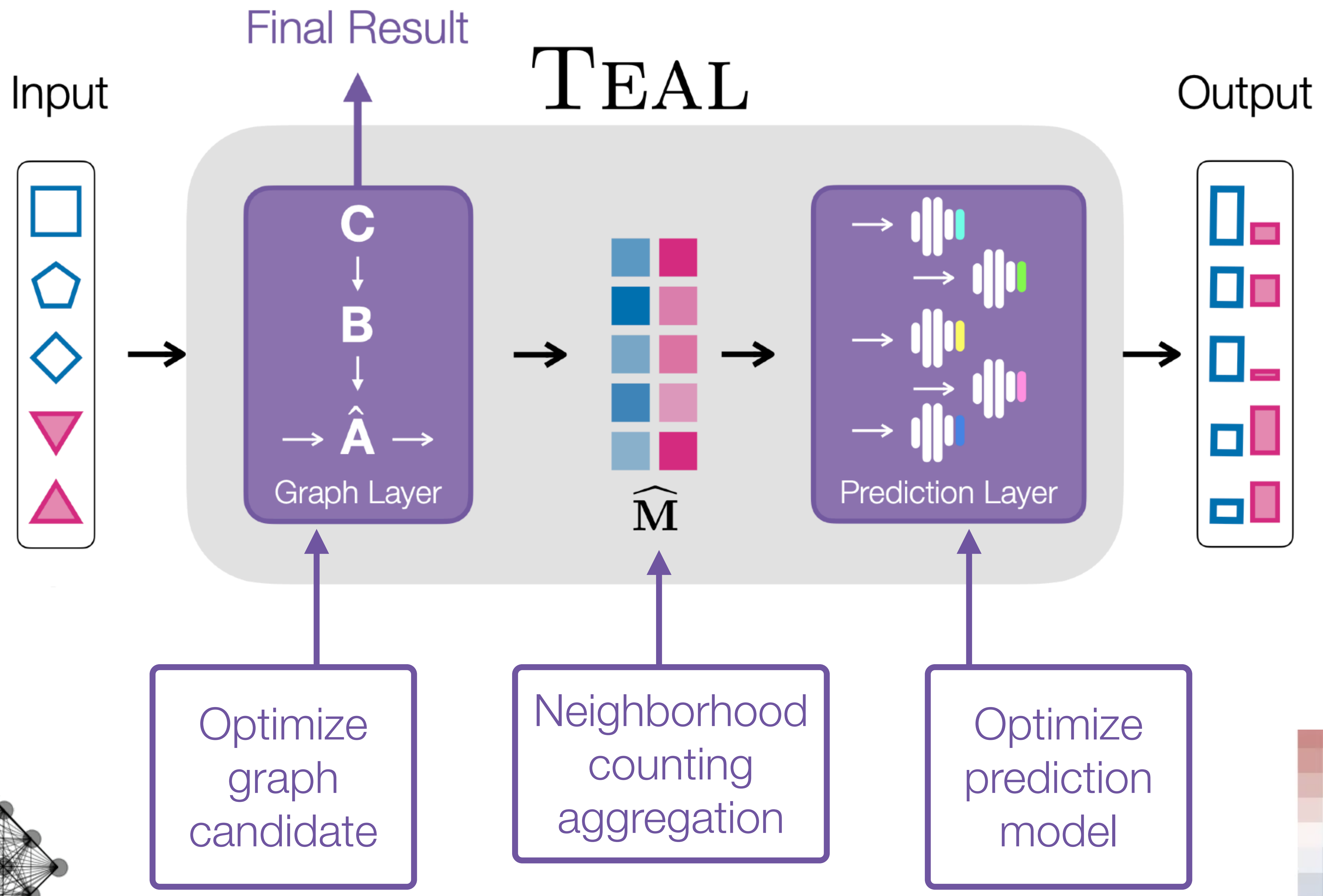

Input
TEAL
Output
1. Mask each node-state.
2. Recover each node-state.

Our Method


Final Result
TEAL
Input
Output
C
B
Â
Graph Layer
M̂
Prediction Layer
Optimize graph candidate
Neighborhood counting aggregation
Optimize prediction model



Our Method



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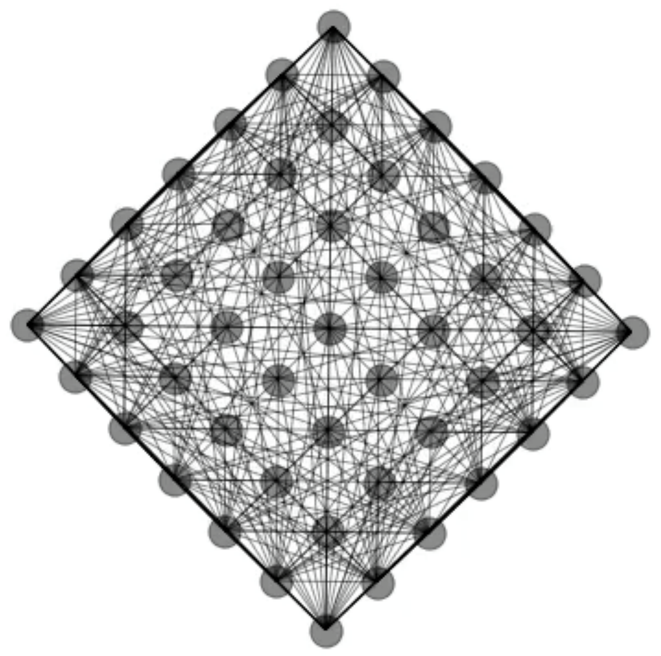
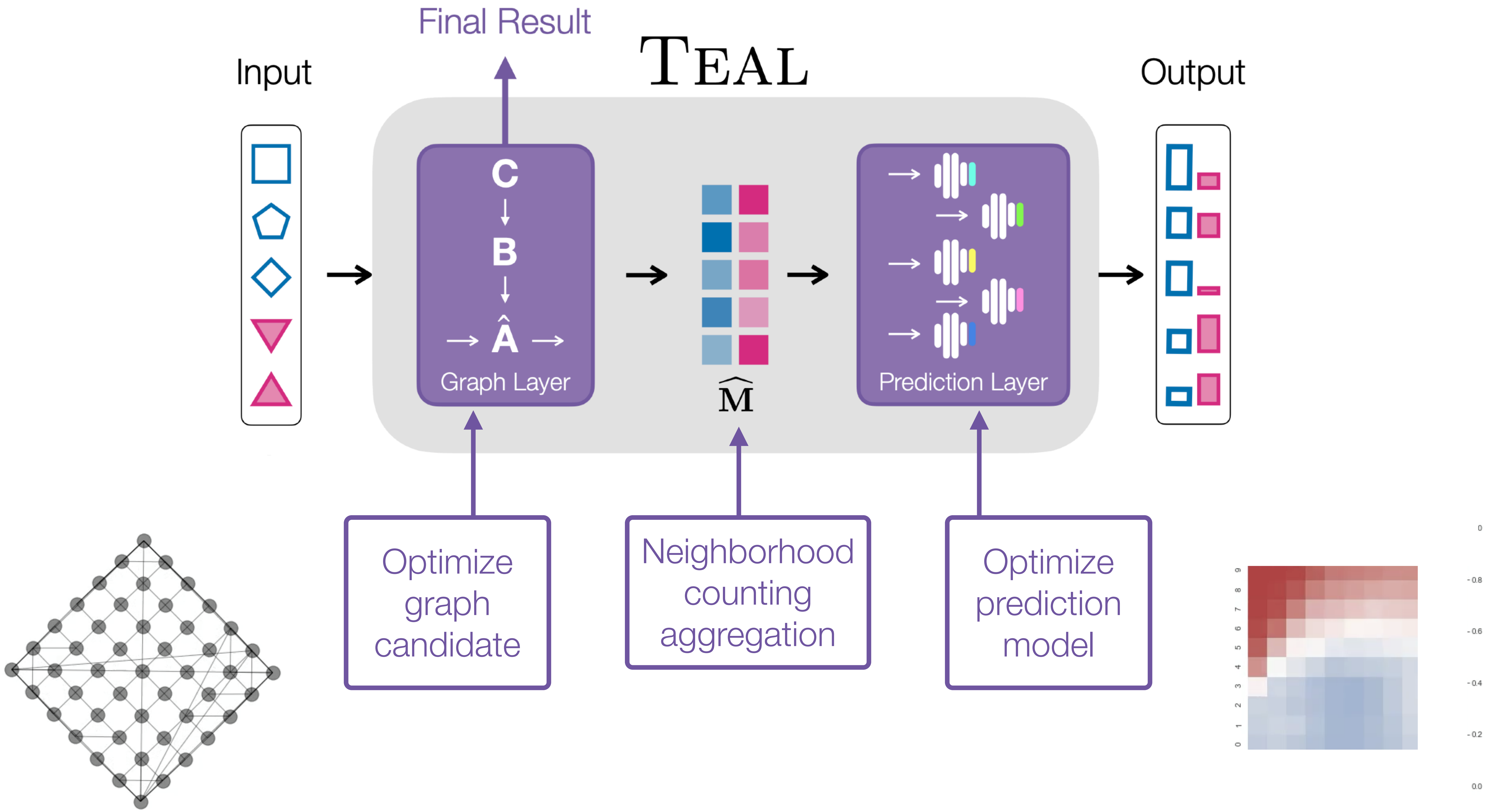


Our Method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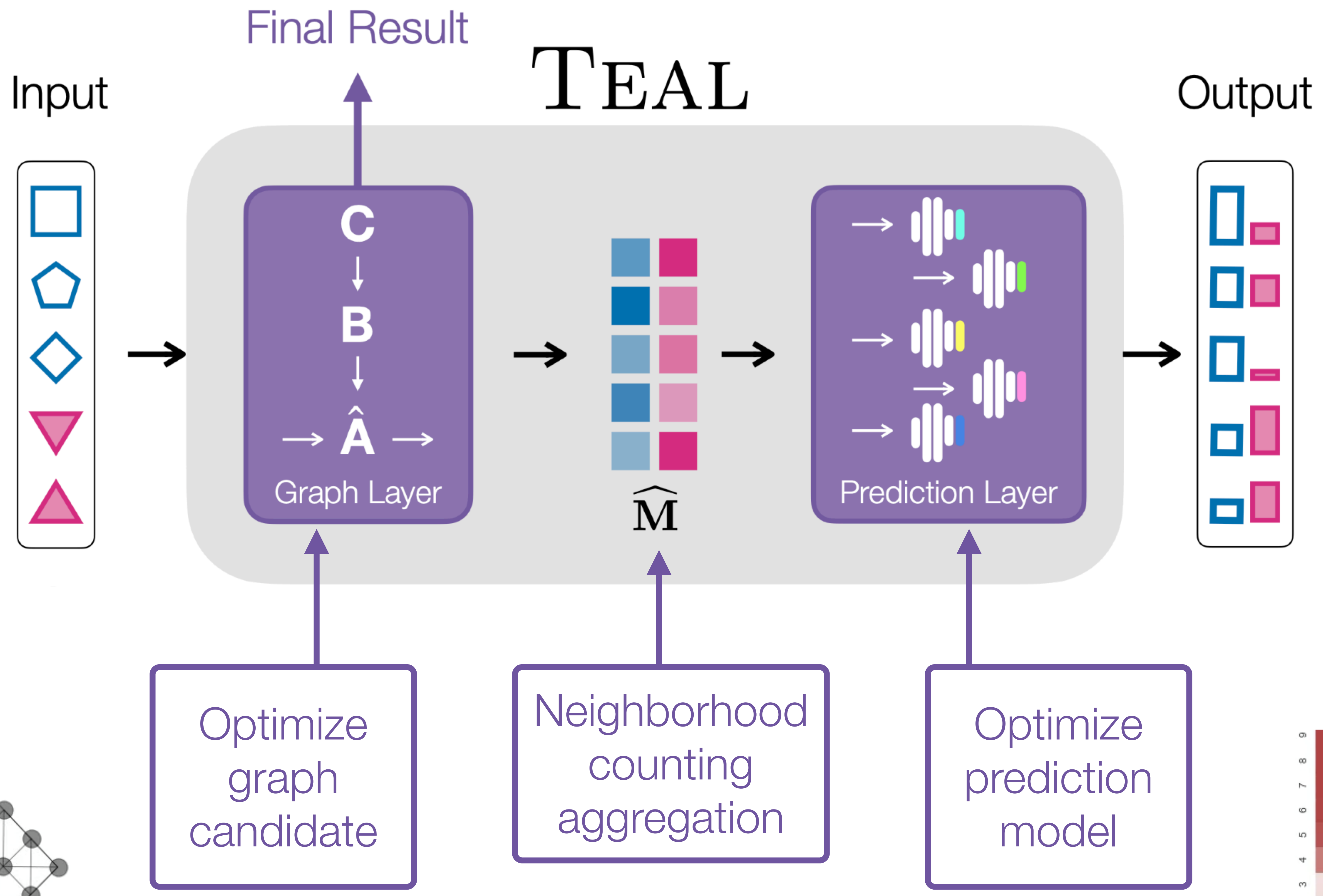

Final Result
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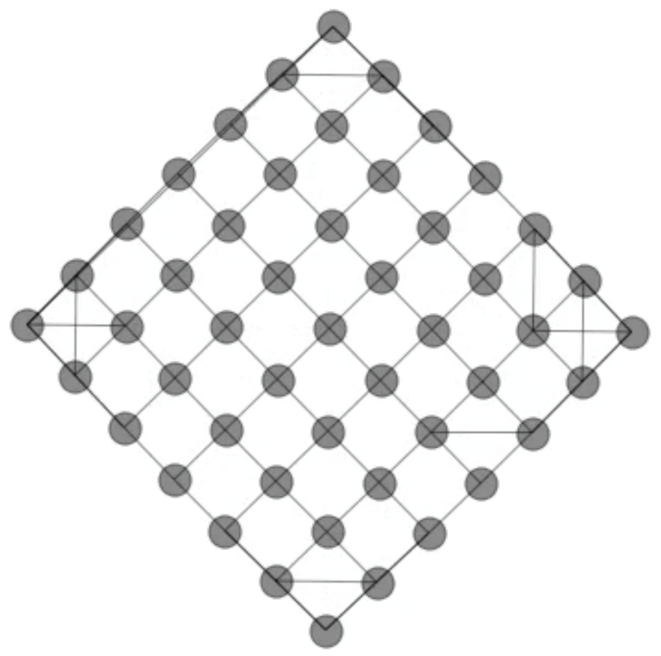
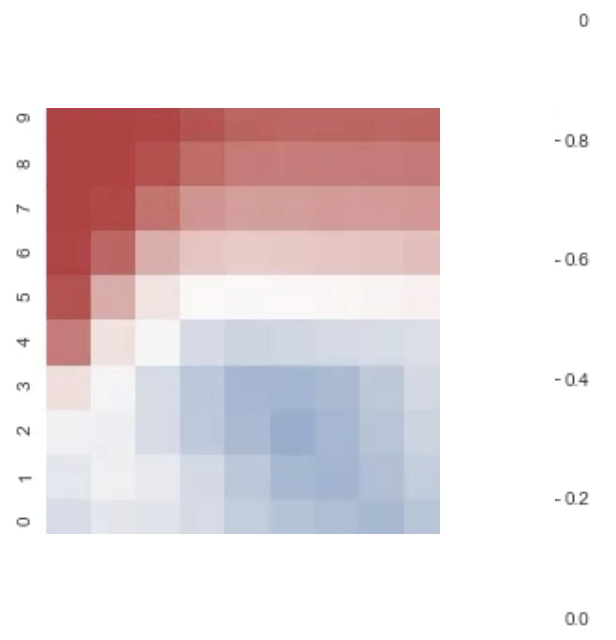
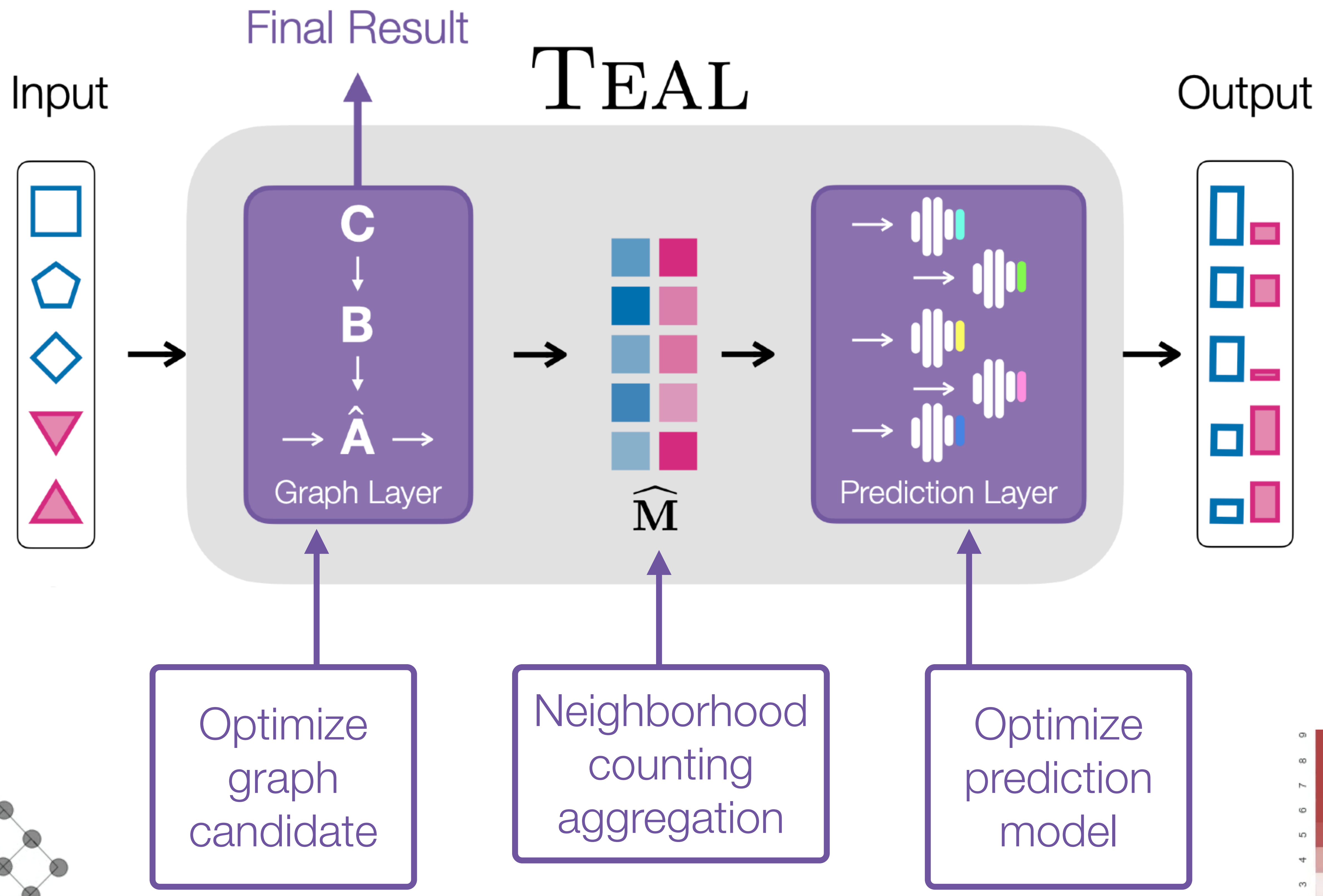




Our Method



Final Result
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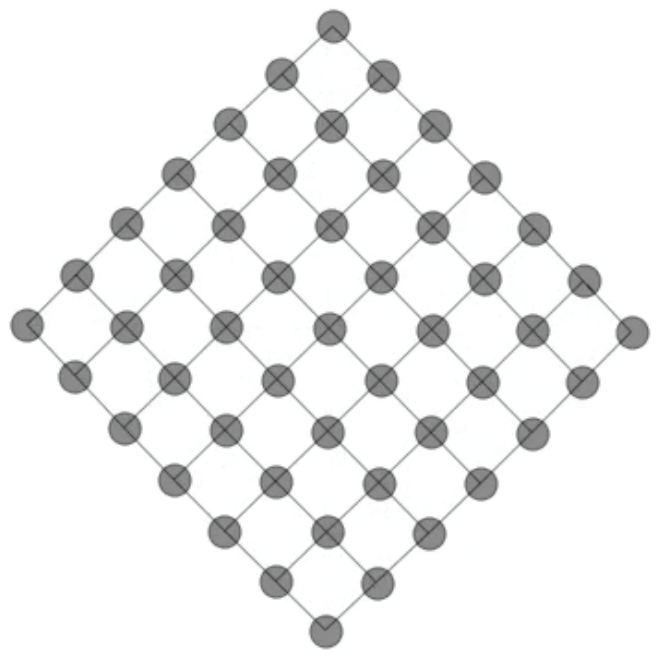
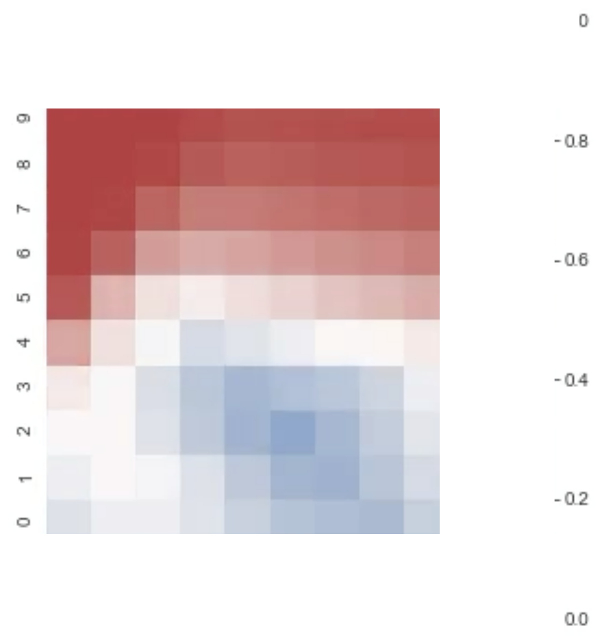
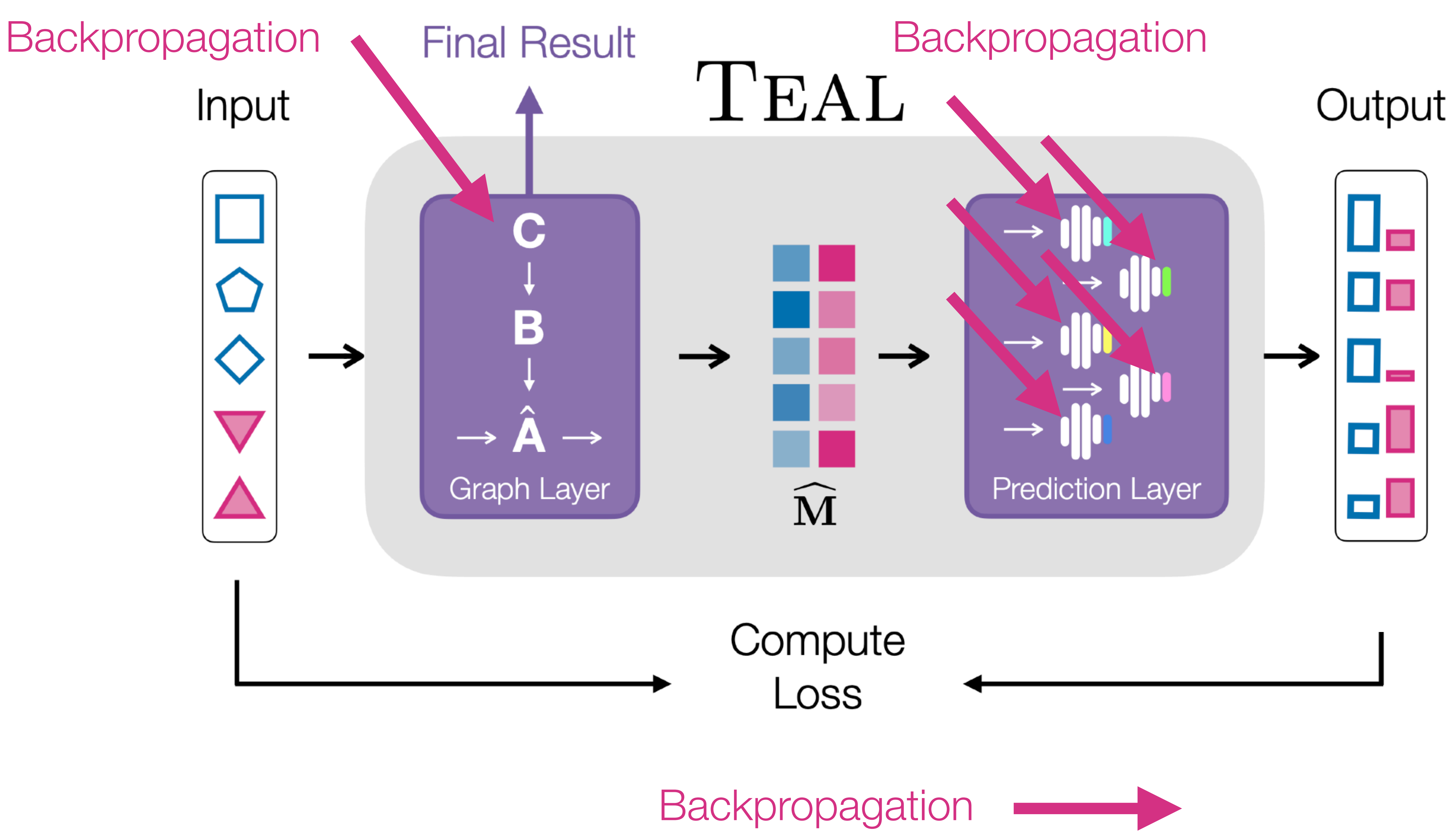
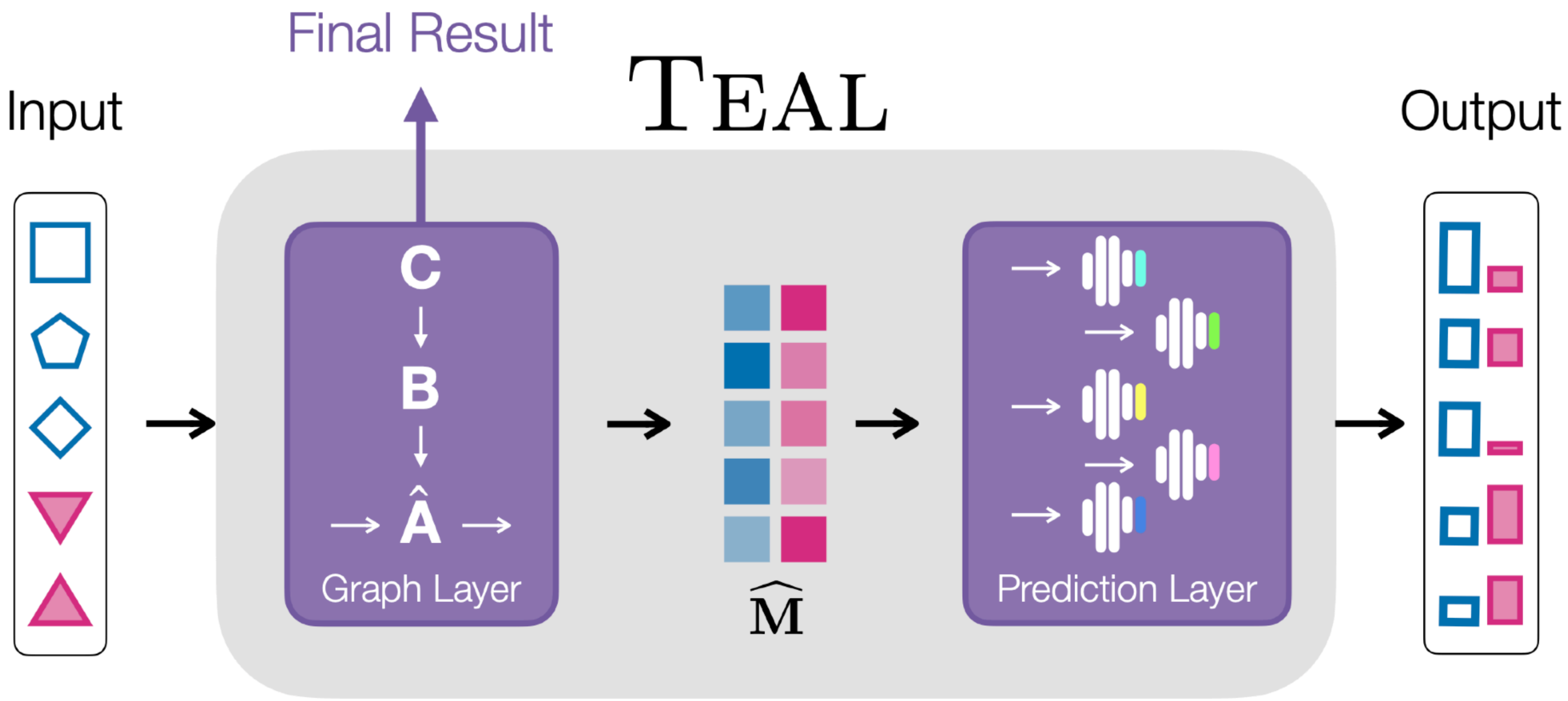




Our Method


Backpropagation
Final Result
TEAL
Backpropagation
Input
Output
C
B
Â
Graph Layer
M̂
Prediction Layer
Compute
Loss
Backpropagation

Our Method

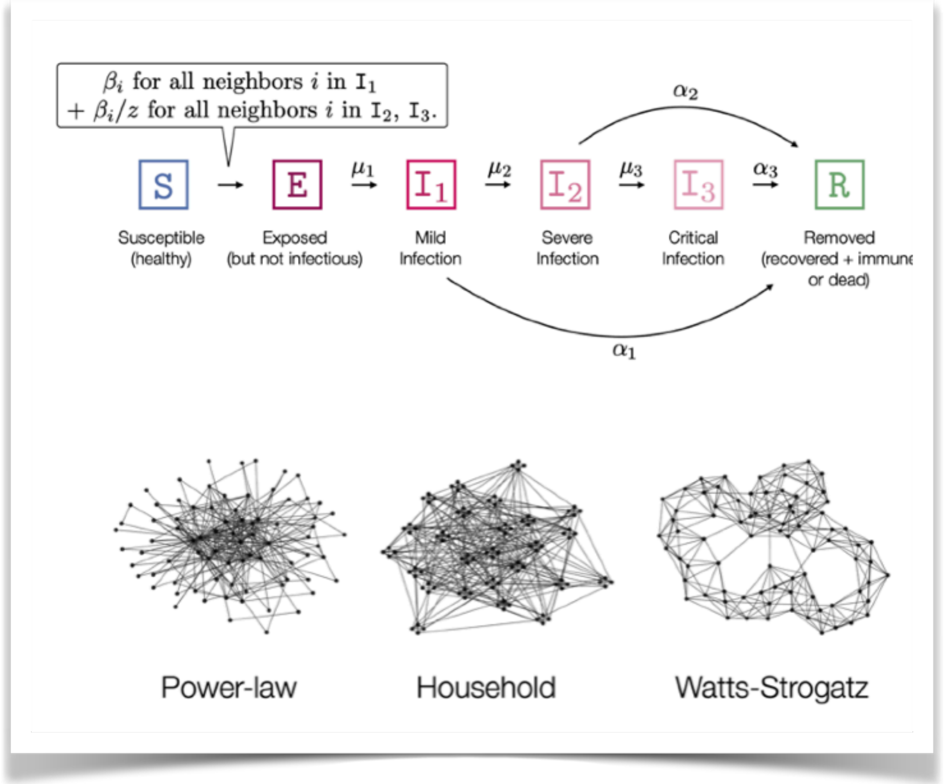


- **Masked reconstruction quantifies** which graph "*best describes*" observed data.
- **Tame vast search space** using SGD.
- **Model-free** and threshold-free network inference;
- **Outperforms** statistical and machine learning baselines.

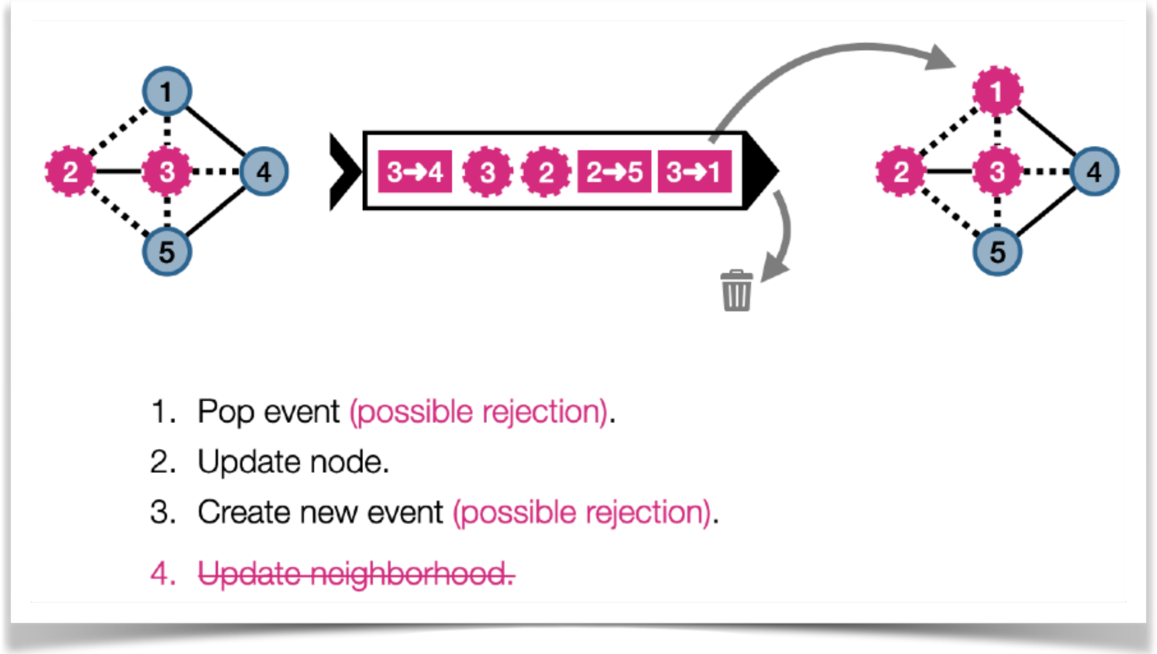
Epilogue

CONCLUDING REMARKS

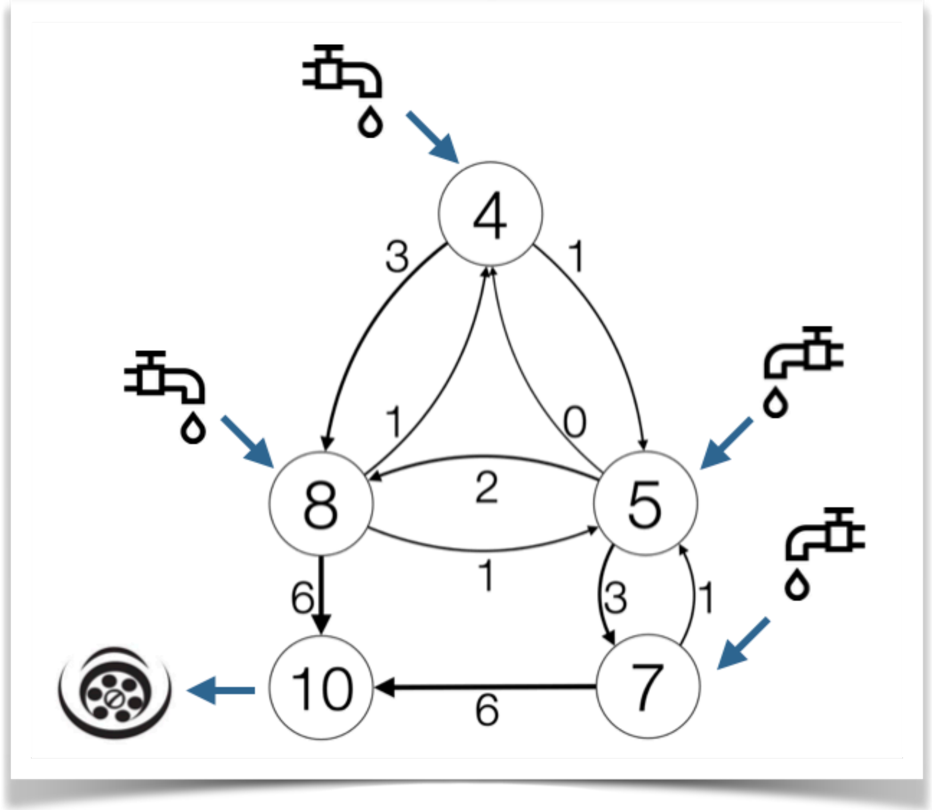
Lessons Learned



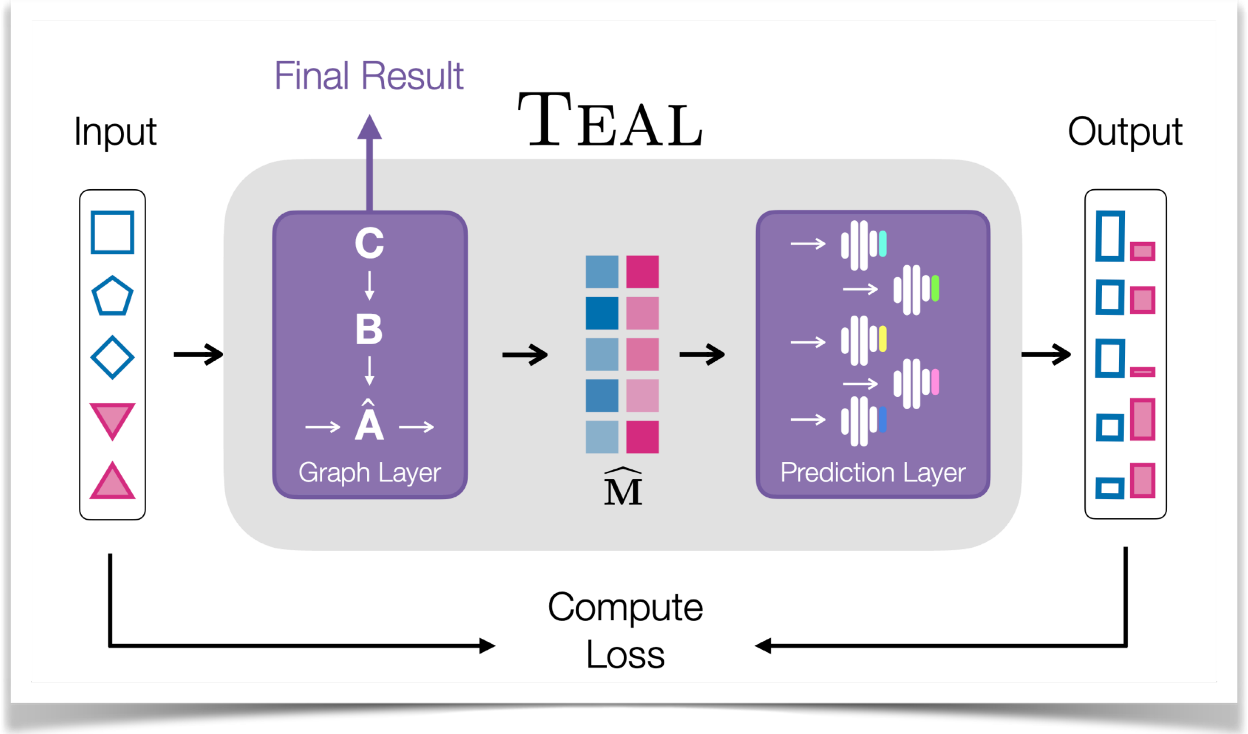
Networks are necessary.



Rejections create chances.

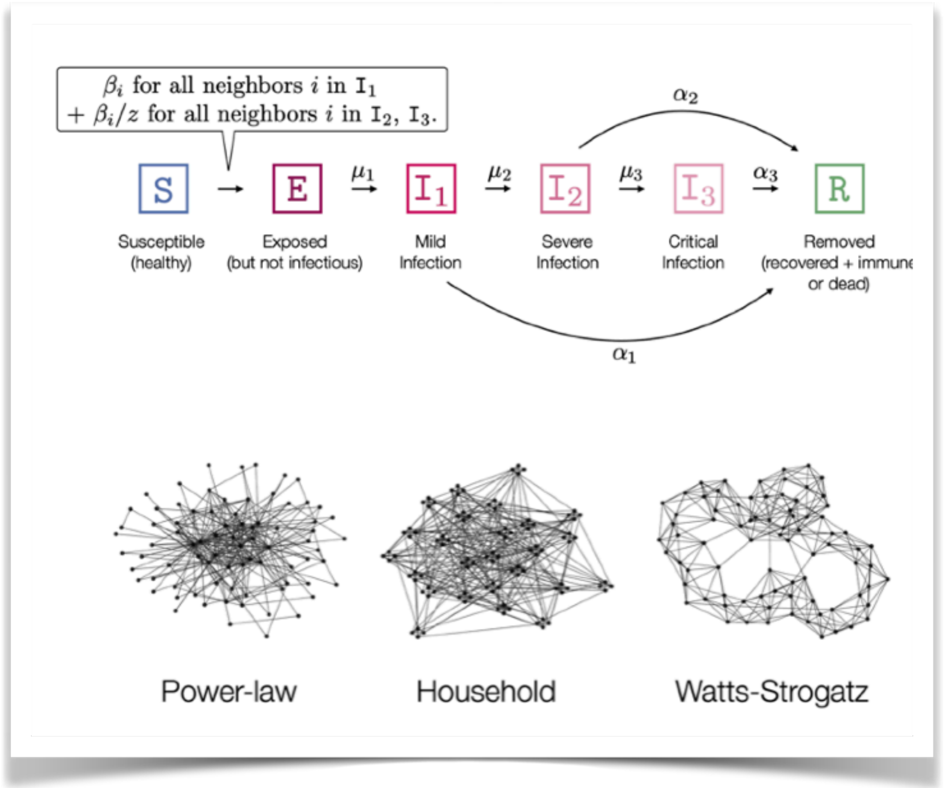


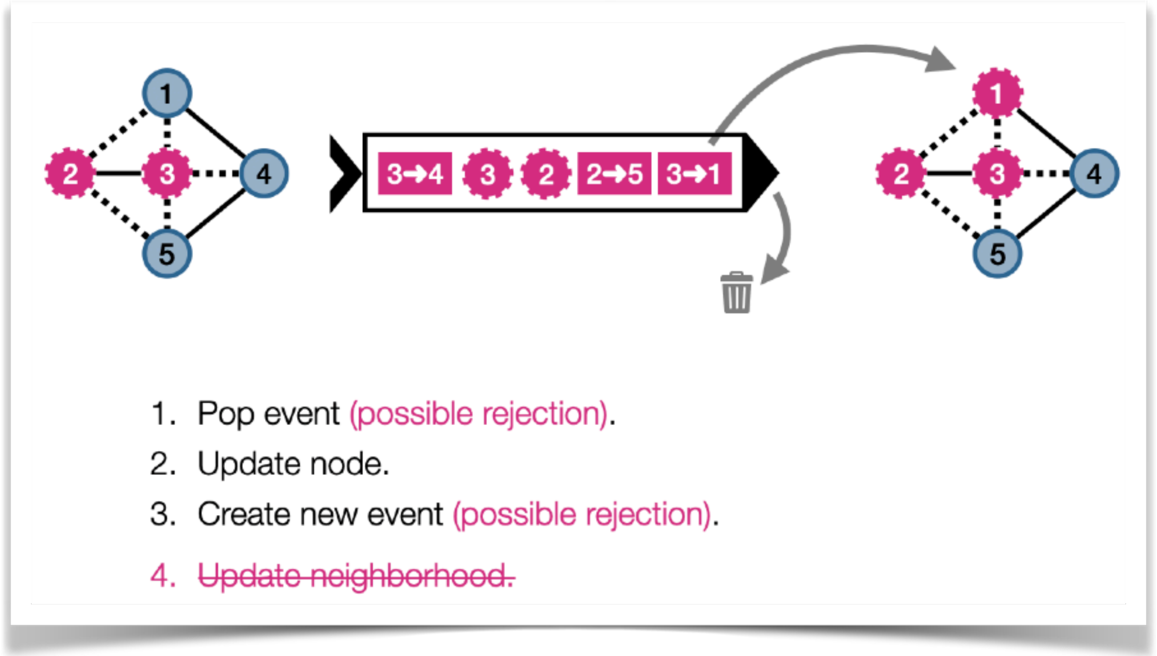
Flow uncovers importance.

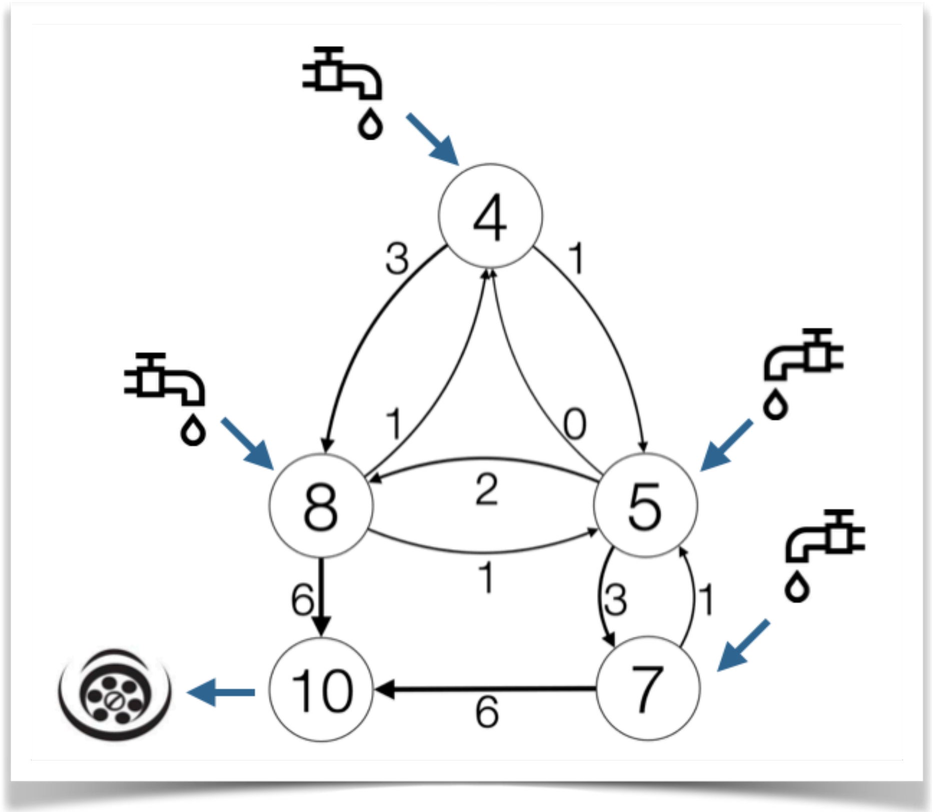


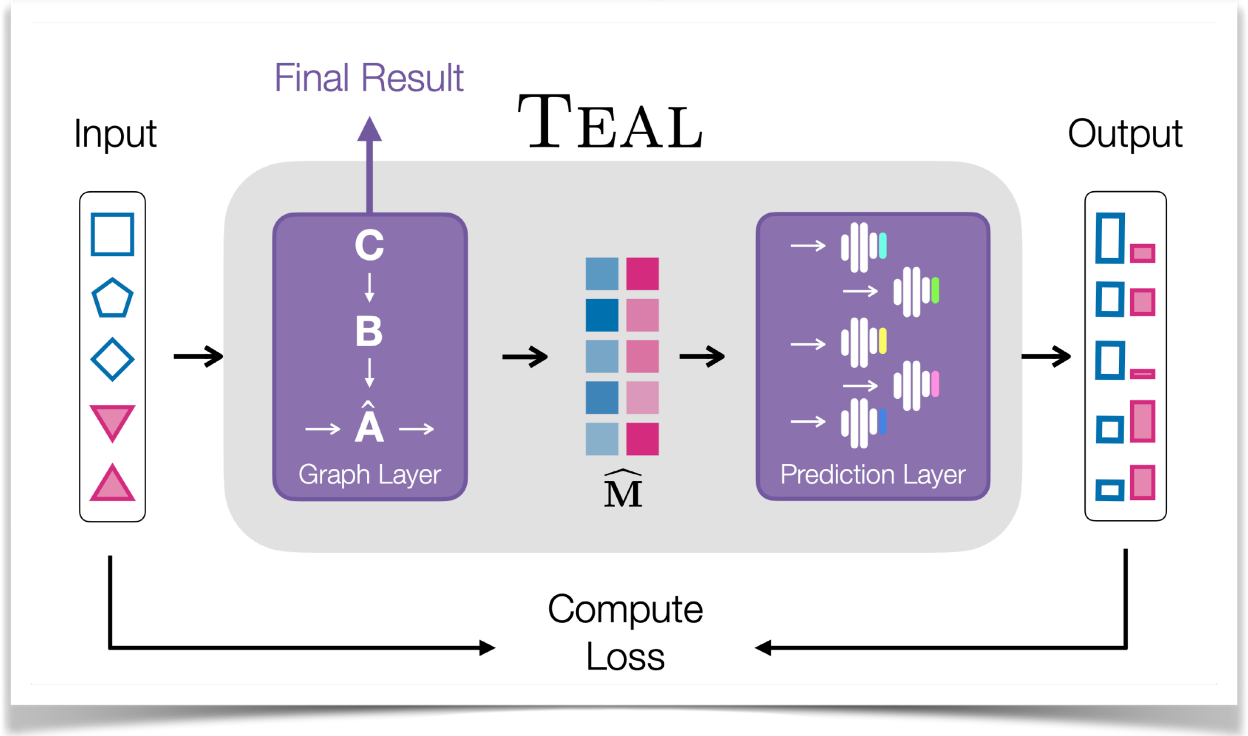
Masking enables inference.

Lessons Learned









Networks are necessary.

Rejections create chances.

Flow uncovers importance.

Masking enables inference.

Future Challenges

- **Obvious extensions:** temporal + adaptive + multilayer + higher order networks
- **Summary statistics:** Something better than prevalence plots?
- **Theoretical challenges:** Mean-field approximation for non-Markov. models
- **Uniform view on emergence:** SIS + Ising model + spin glass + point processes + percolation theory