Network Reliability: a Generic Tool to Explore Diffusive Processes on Interacting Systems

NASA PCE3 Virtual Workshop 2022 Nano-to-Cosmic Studies of Complex Systems

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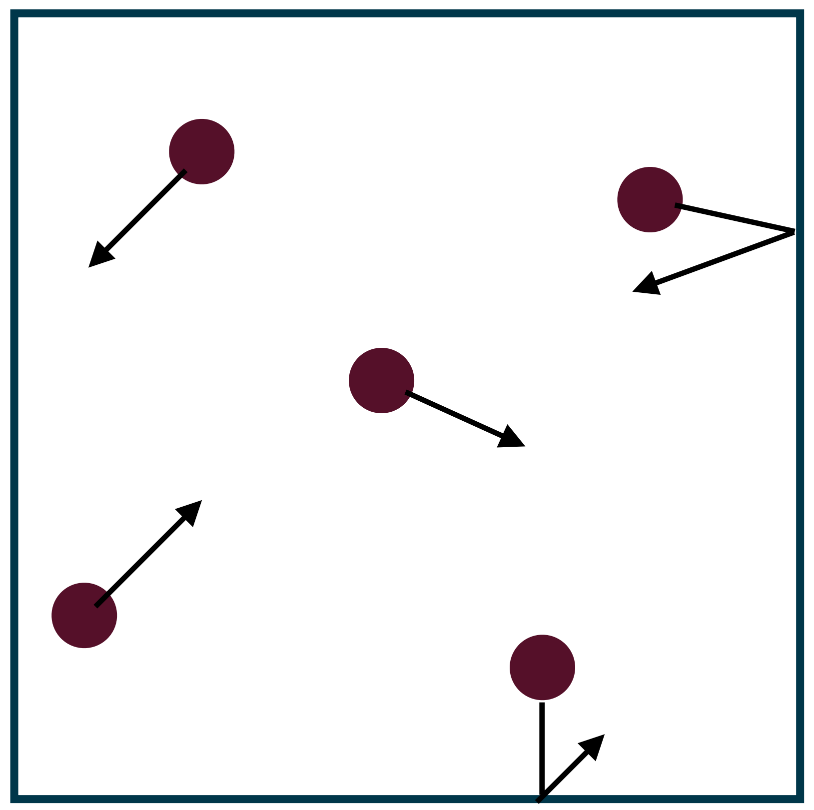
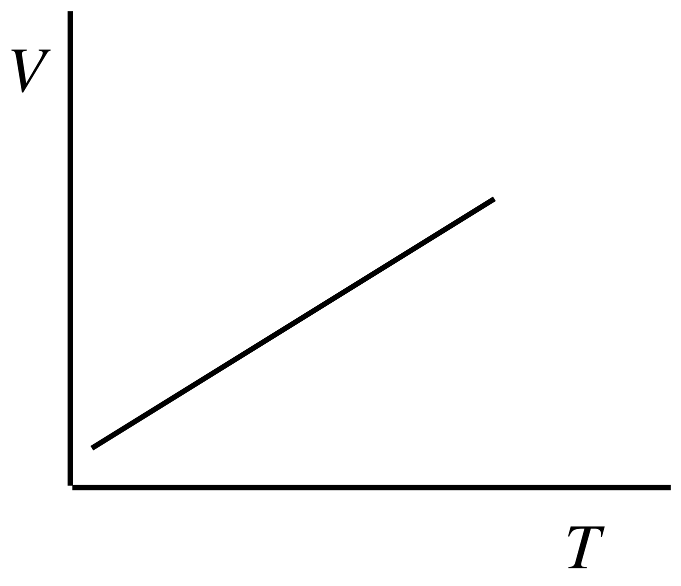
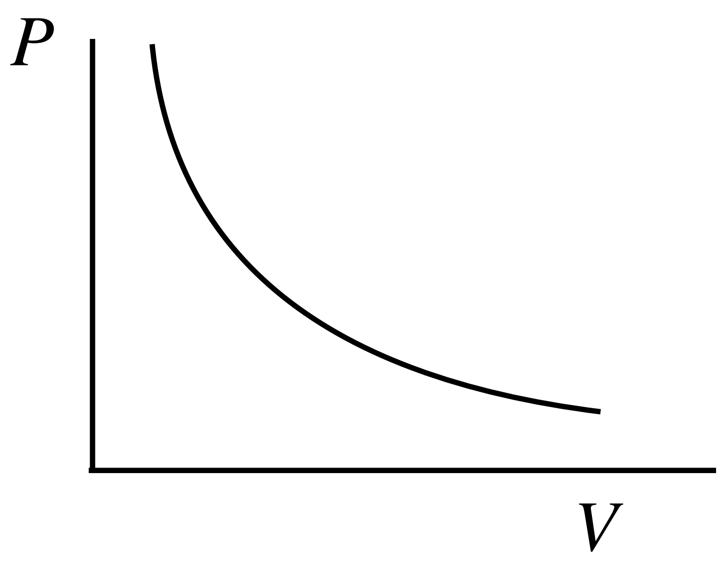
Models of Ideal Gas

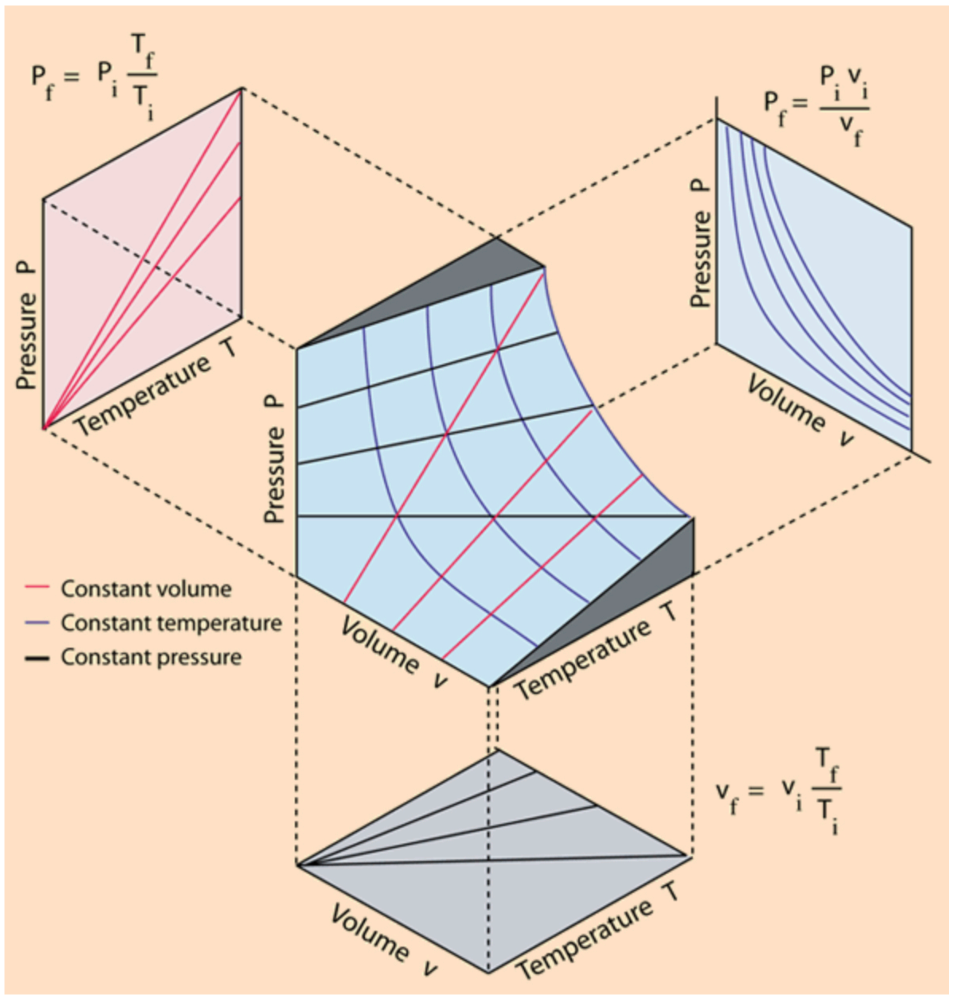
In physics, to explain and understand a phenomenon or a process, we often start with a *simple model* before adding perturbations or other higher order interactions.

On the other extreme, we know exactly how to deal with thermodynamic limit in a ordered system, or limit $\to \infty$.









Kinetic theory:

molecules $\leftrightarrow$ billiard balls (microstates)

Equations of state:

$PV \propto T, \quad V \propto T$

(macrostates)

Kinetic Theory $\Longrightarrow$ Ideal Gas Equation:

$PV = nRT$ - Krönig (1856) & Clausius (1857)

<u>Micro to Macro synthesis</u>

http://hyperphysics.phy-astr.gsu.edu/hbase/Kinetic/idegas.html

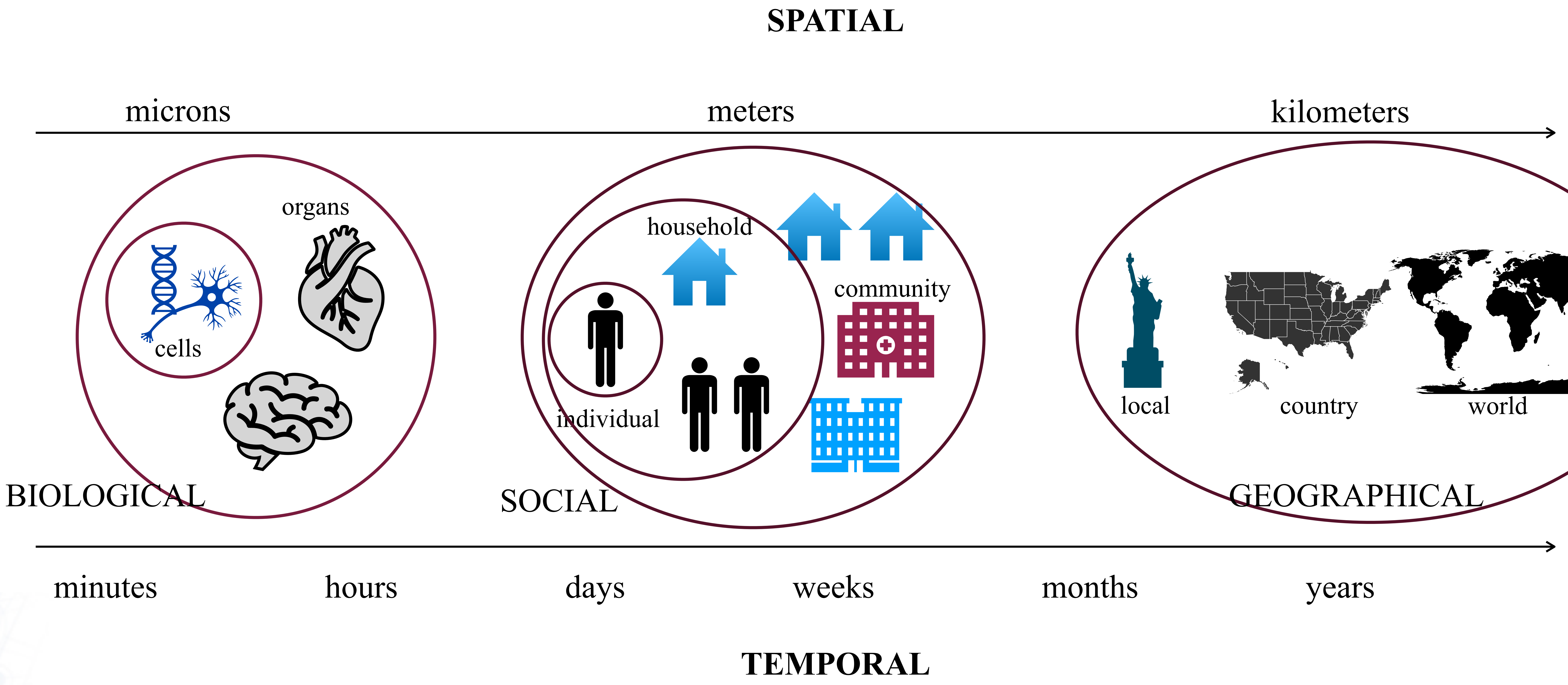
Passing from the ideal to the real

Real-world scenarios arise due to **many-body interactions**, and they are not often in a regular/ordered state → becomes extremely hard to extract the required information.

- no well-defined boundaries
- no regularity, symmetry, smoothness
- no Gaussian or unimodular distribution
- no asymptotic behaviour
- no scale separation
- $10 \ll N \ll 10^{23}$

Passing from the ideal to the real

Problems in real world are **messy**.



Why complex systems are interesting?

COMPLEX NETWORKS/GRAPH THEORY

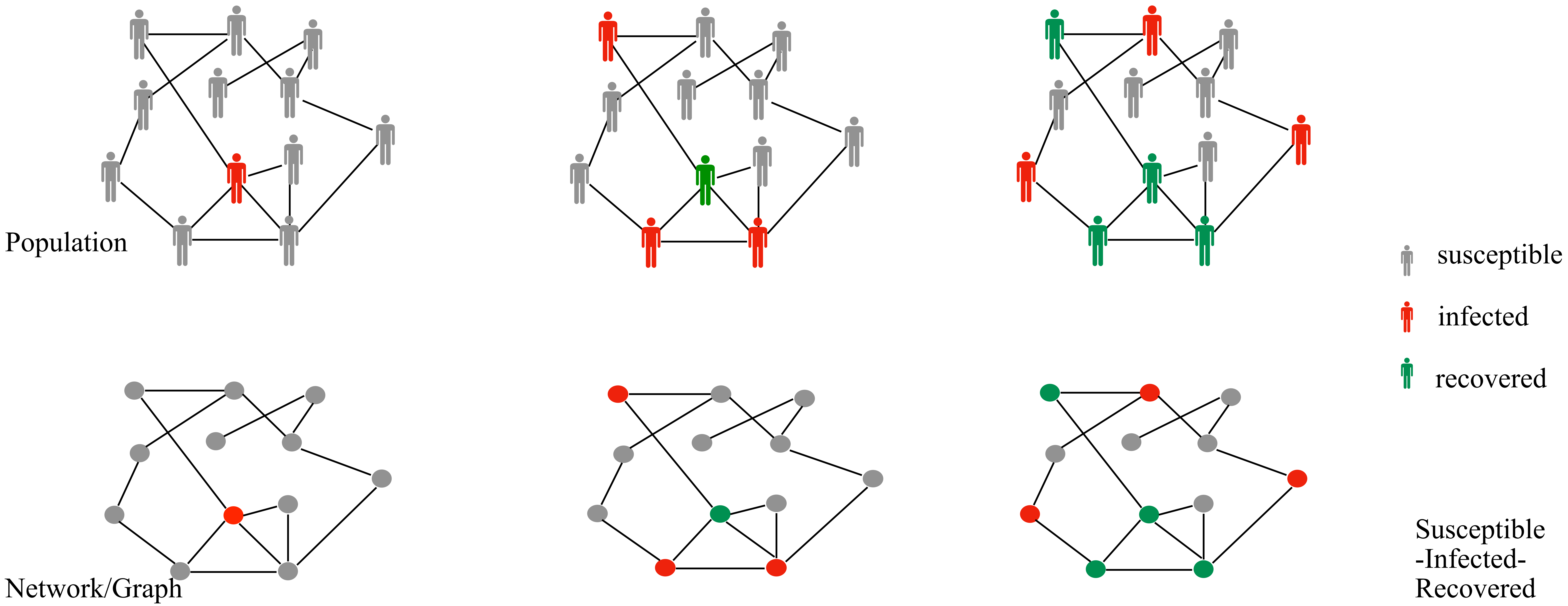
Applications ranging from biology to social sciences to engineering to machine learning.

The **Nobel Prize in Physics 2021** was awarded "**<u>for groundbreaking contributions to our understanding of complex physical systems</u>**" with one half jointly to Syukuro Manabe and Klaus Hasselmann "for the physical modelling of Earth's climate, quantifying variability and reliably predicting global warming" and the other half to Giorgio Parisi "for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales".

The Nobel Prize in Physics 2021. NobelPrize.org. Nobel Prize Outreach AB 2022. Tue. 11 Oct 2022

Spread of an infectious disease can be studied using networks to take preventive measures

Application



Susceptible
-Infected-
Recovered
(S-I-R)
process

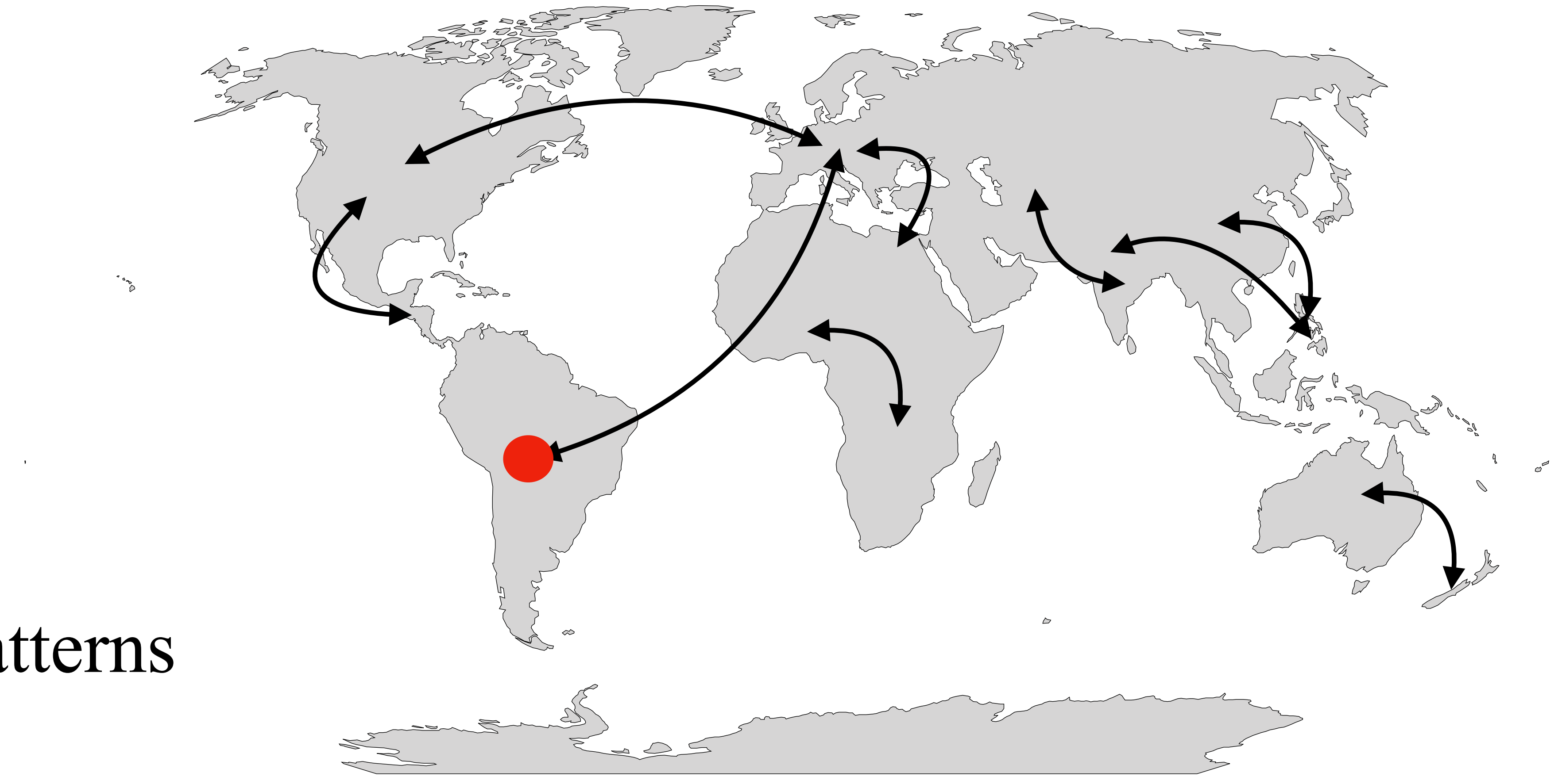
Propagation of Infectious Diseases ⟷ Dynamics

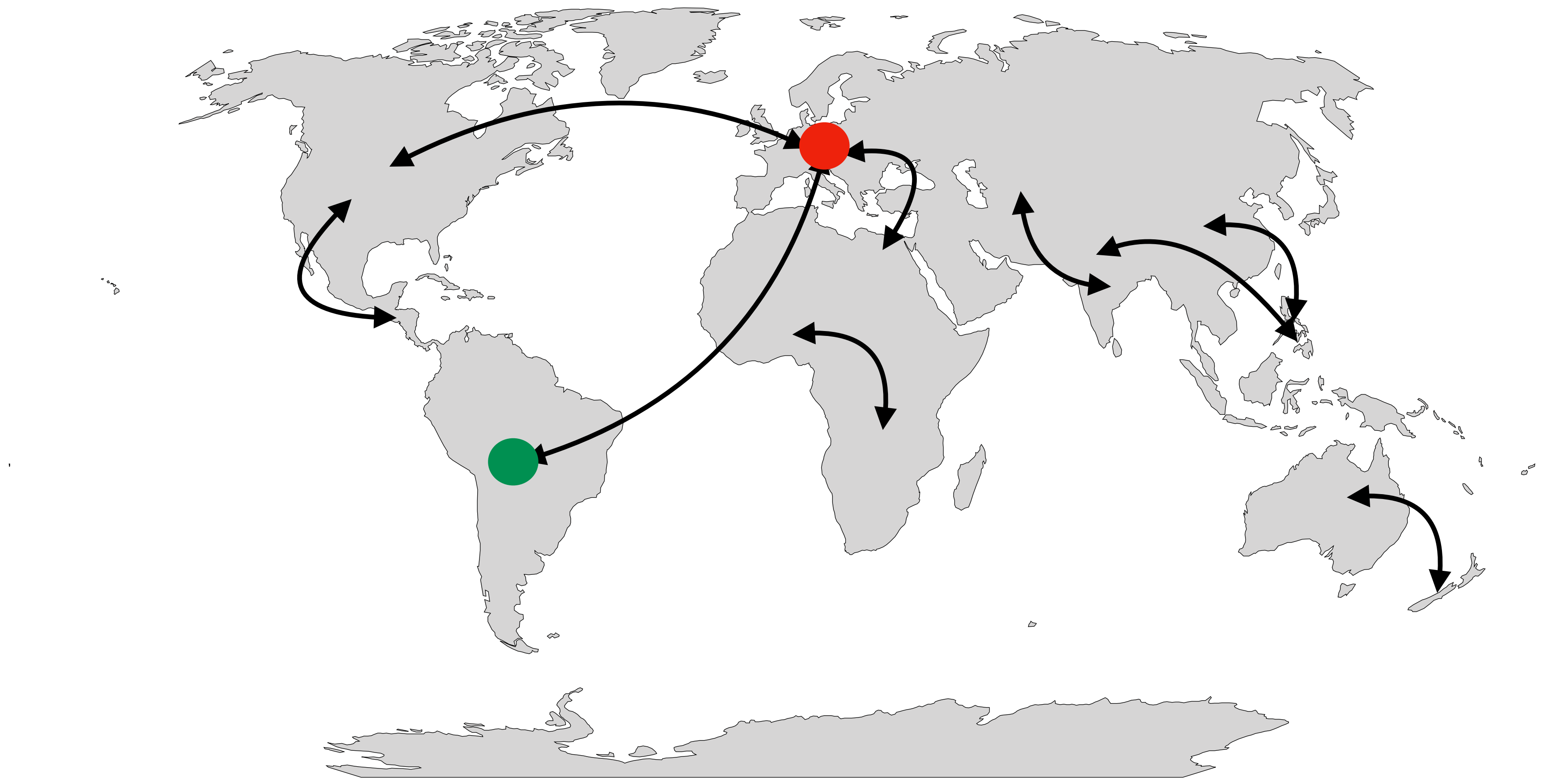
Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Spread of a pest affecting crops can be studied using networks to take preventive measures

Application

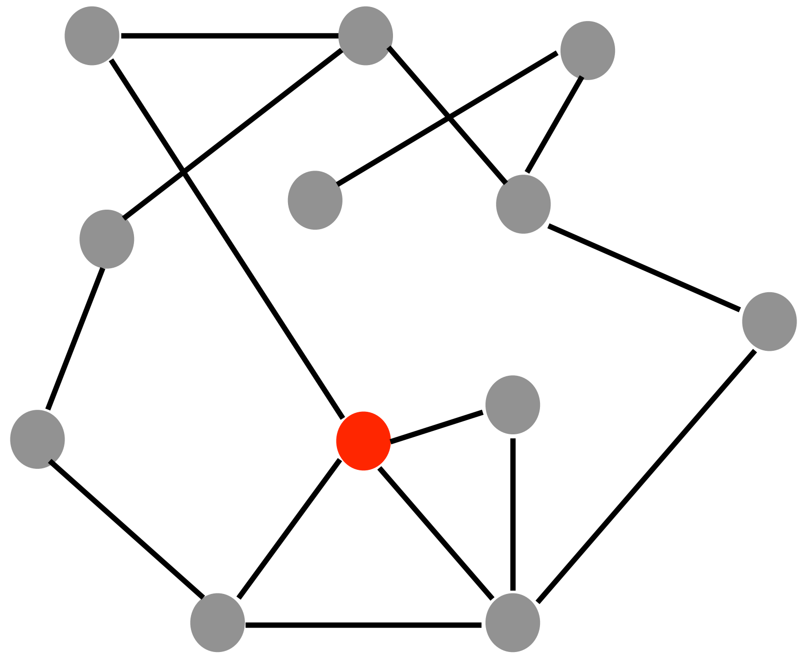
Trade Patterns

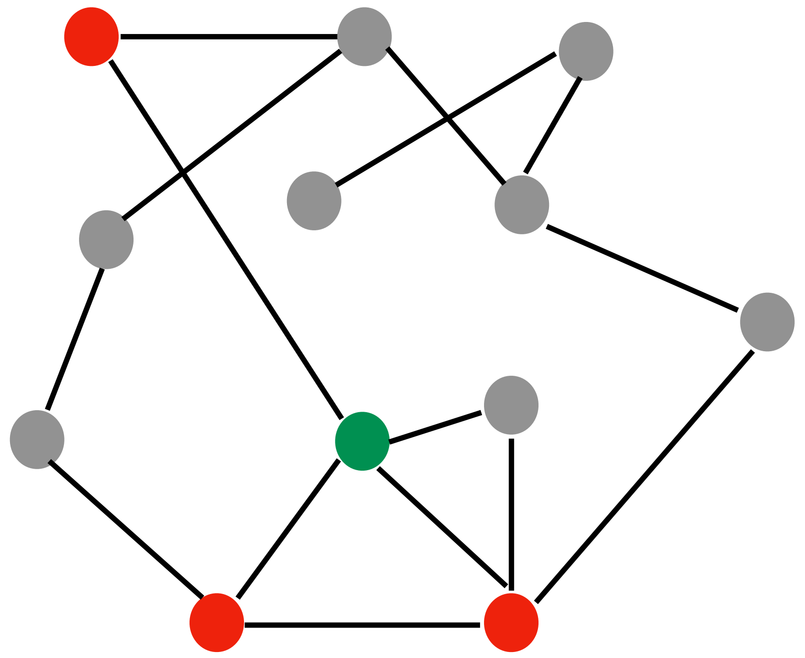




- susceptible
- infected
- recovered

Network/Graph





Susceptible-Infected-Recovered (S-I-R) process

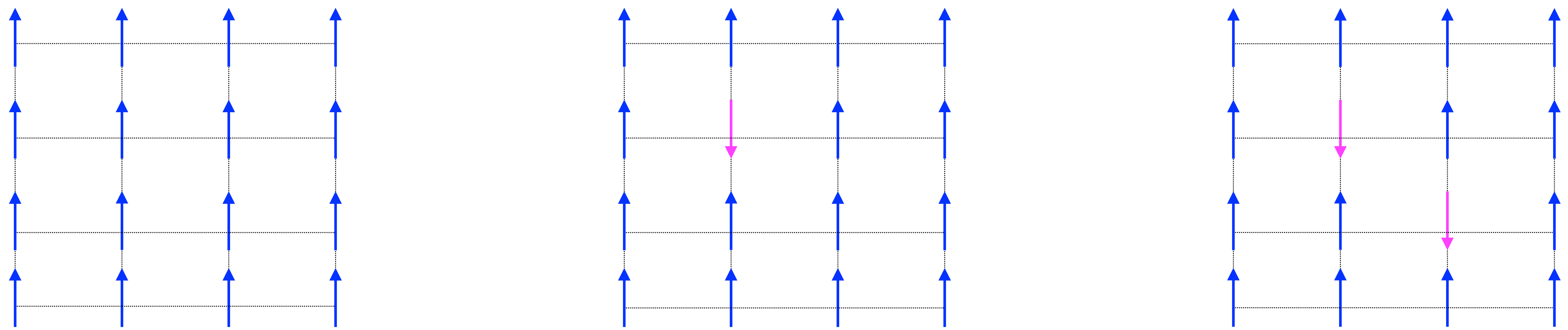
Propagation of Pest/Invasive Species ⟷ Dynamics

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

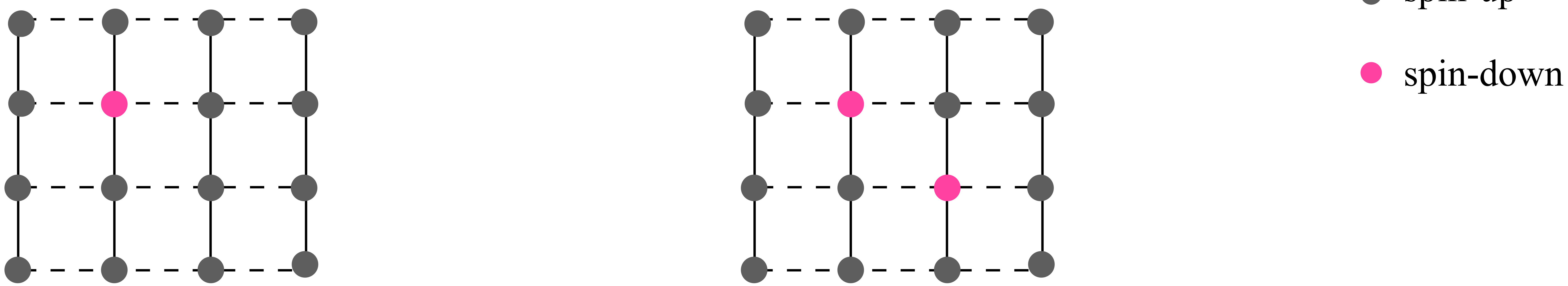
The Ising model in an external field can be studied using networks to understand physical systems

Application

Lattice



Network/Graph



Propagation of Spin Flips ⟷ Dynamics

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

What is the probability that a finite sized interacting system in a specific configuration now will have a certain property later?

- given a lattice of magnets free to flip their orientations, what is the probability that two magnets separated by k lattice sites point in the same direction?

- given an infected individual in a susceptible population, what is the probability of observing an epidemic outbreak?

- given a network, what is the probability that a path exists between two points, Source S and Terminal T?

- given the probability of failure for “crummy” relays in an electrical circuit, what is the probability of establishing a current from one terminal to another?

- given a network, identify a set of vertices/edges that has the most influence on the dynamics

Eubank, S., et. al., Perturbative methods for mostly monotonic probabilistic satisfiability problems. arXiv preprint arXiv:2206.03550, 2022.
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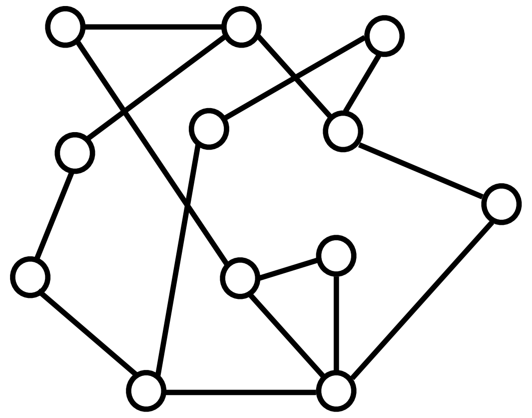
Graph dynamical system and Moore-Shannon network reliability are general formalism

<u>Network reliability</u> *is* the probability that a finite sized graph dynamical system in a specific configuration now will have a certain property later.

Graph Dynamical System (GDS)
- provides a formal model to capture the structure and the dynamics.
- interacting system mathematically represented by a graph having vertices/nodes and (un)directed/(un)weighted edges.
- represent any system of discrete nodes whose state changes according to their interactions with neighbours, does not assume any regularities or symmetries in the structure of the network.



Network reliability finds **a path between two nodes**, **estimates epidemic potential**, **detects differences in the dynamics** due to differences in **network structure**, **recalibrates networks** with different structure and **identifies strongly connected clusters**.

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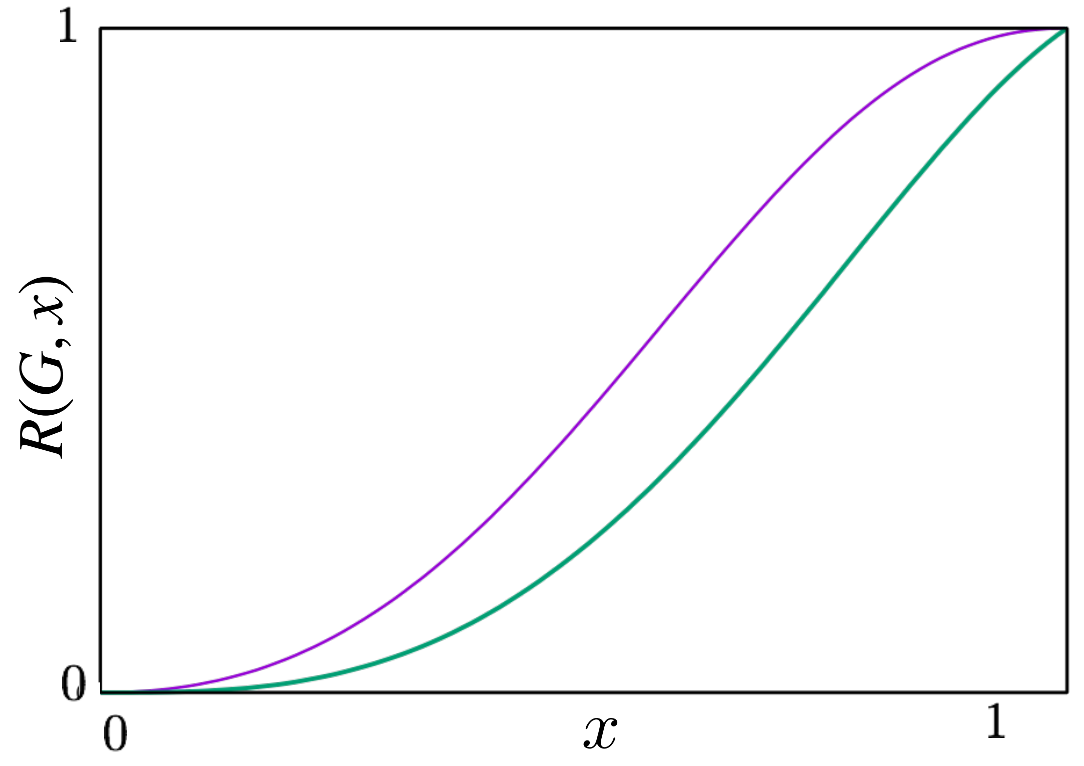
Why Moore-Shannon network reliability?

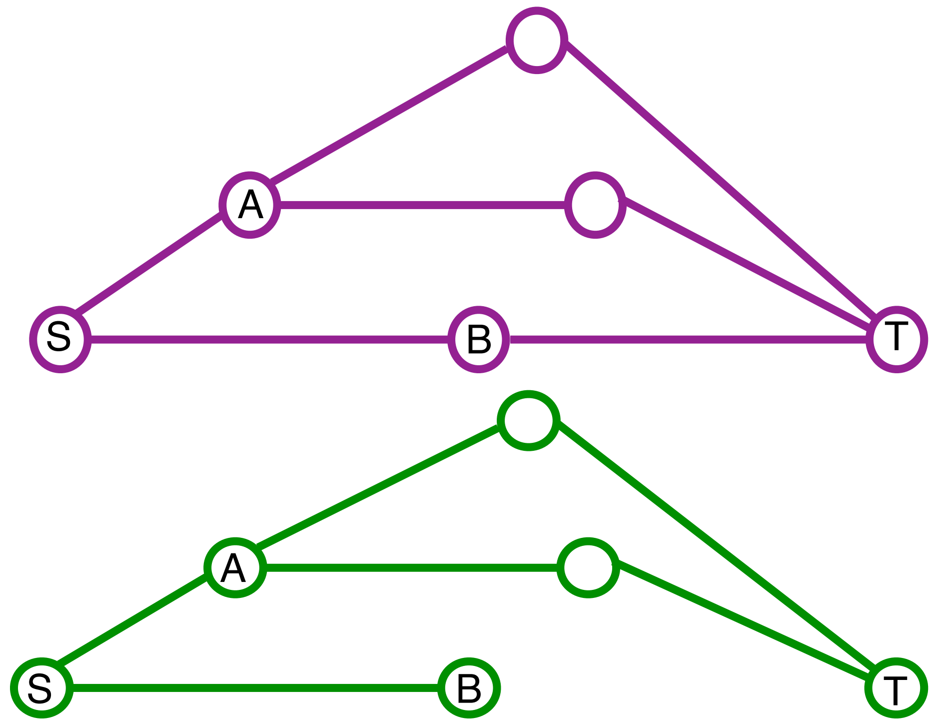
- A **function of both structural and dynamical** aspects of any system
- A **generic** tool with a wide range of applications
- Can provide a new perspective on some old problems
- Related to partition function of a system (statistical physics)

In a system with a finite number of configurations,

$n(k) =$ fraction of dynamical paths leading to a configuration with property that have probability p_k

$$p(\mathscr{E}) = \sum_{k \in \mathscr{K}} n(k) p_k \equiv R(G, x) = \text{network reliability}$$





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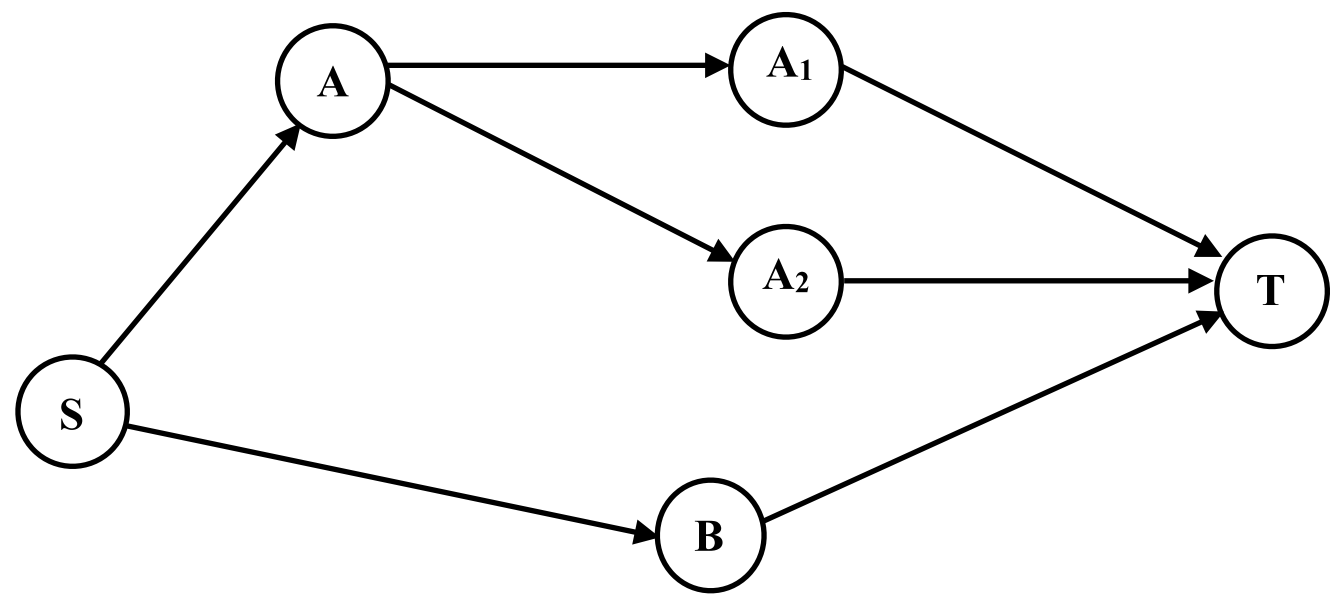
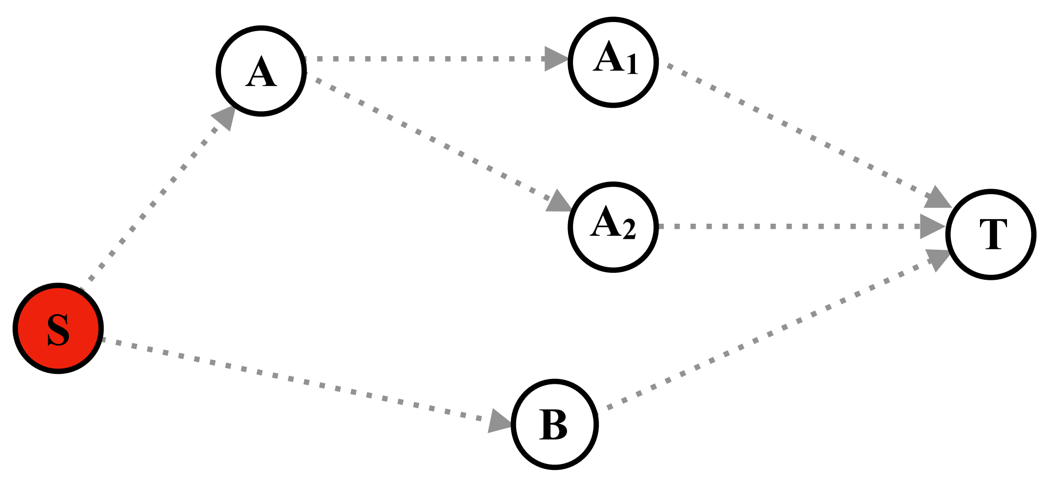
Moore, E., Shannon, C.: Reliable circuits using less reliable relays, Journal of the Franklin Institute 262, 191–208,1956.
Youssef, M., Khorramzadeh, Y., Eubank, S.: Network reliability: the effect of local network structure on diffusive processes, Physical Review E, 88.5: 052810, 2013.

Calculating network reliability for homogenous toy network (1/3)

Key Concepts

Assuming S is infected and others susceptible, what is the probability that T will be infected, i.e., probability that there exists a path between S and T?





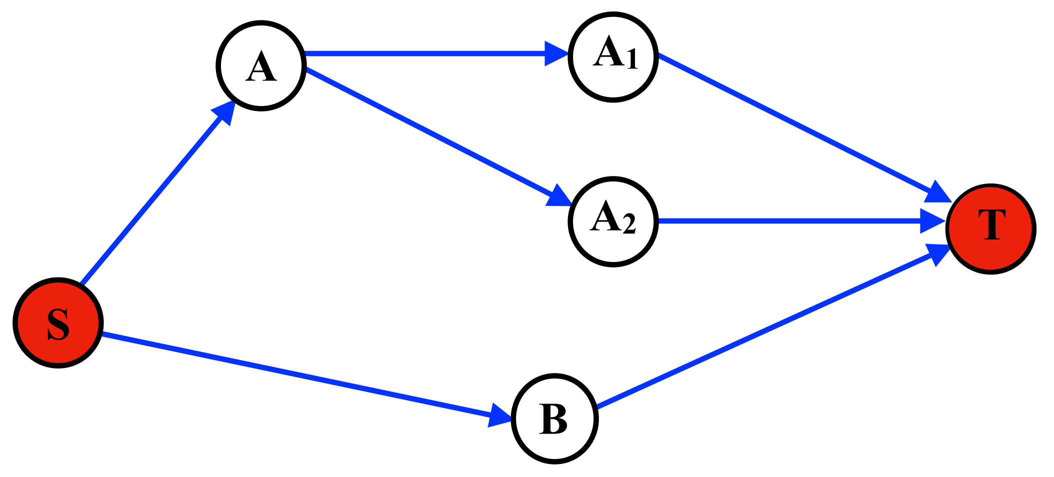
When **no edges** are connected, S and T are not connected

GDS: Graph with 6 nodes and 7 edges

S-I-R dynamics

property: vertices S and T are connected

x = probability of transmission through each edge



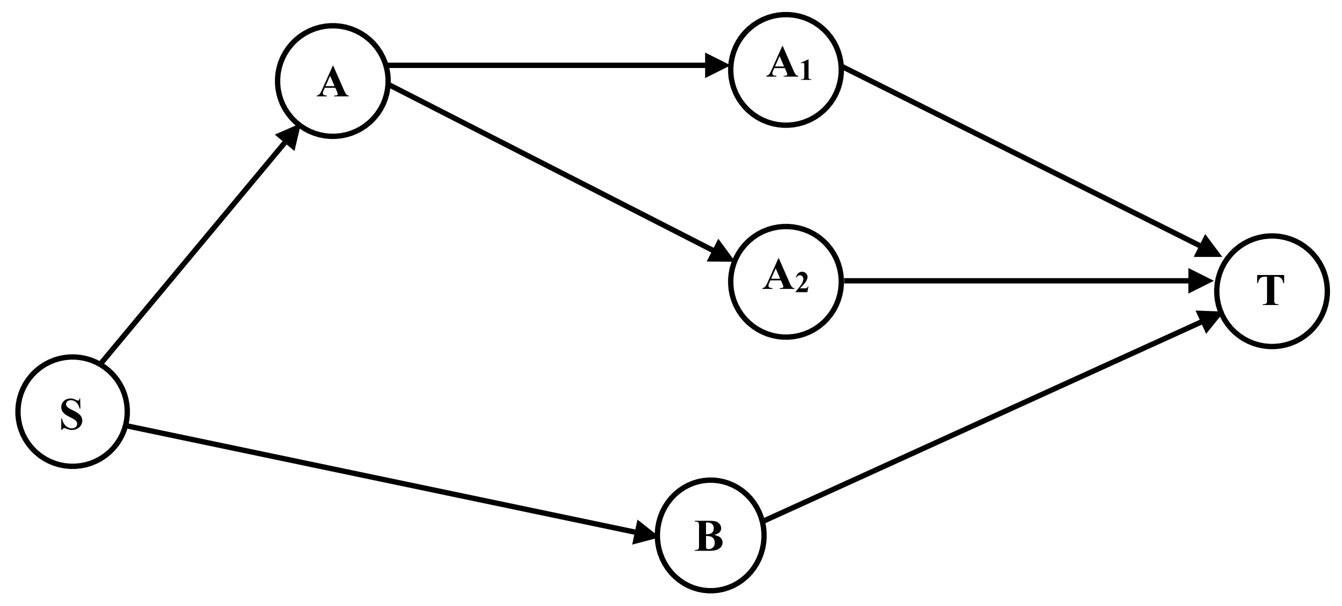
When all **edges** are connected, S and T are connected

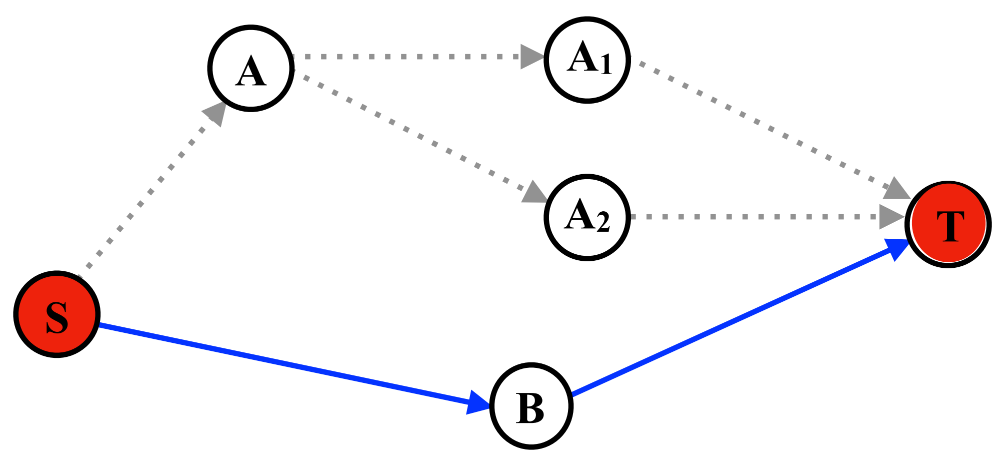
Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Calculating network reliability for homogenous toy network (2/3)

Key Concepts

Assuming S is infected and others susceptible, what is the probability that T will be infected, i.e., probability that there exists a path between S and T?





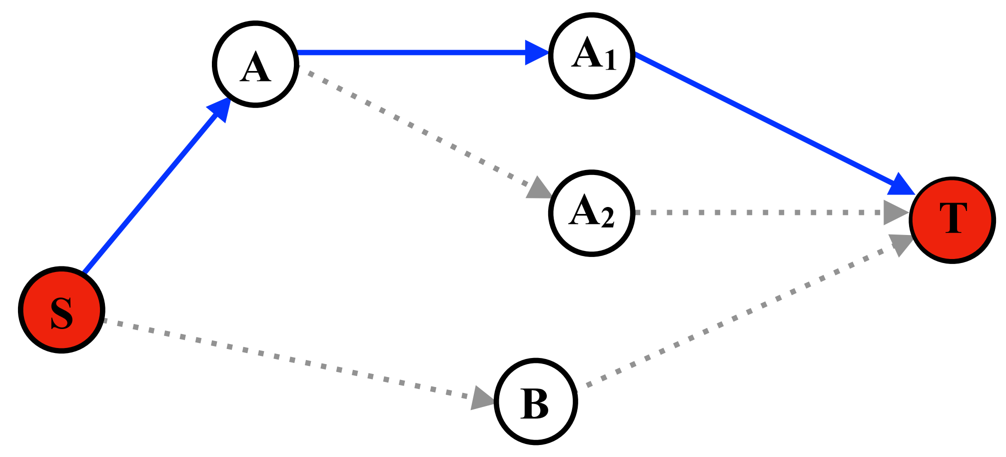
At minimum, **two edges** - SB & BT are required for S and T to be connected

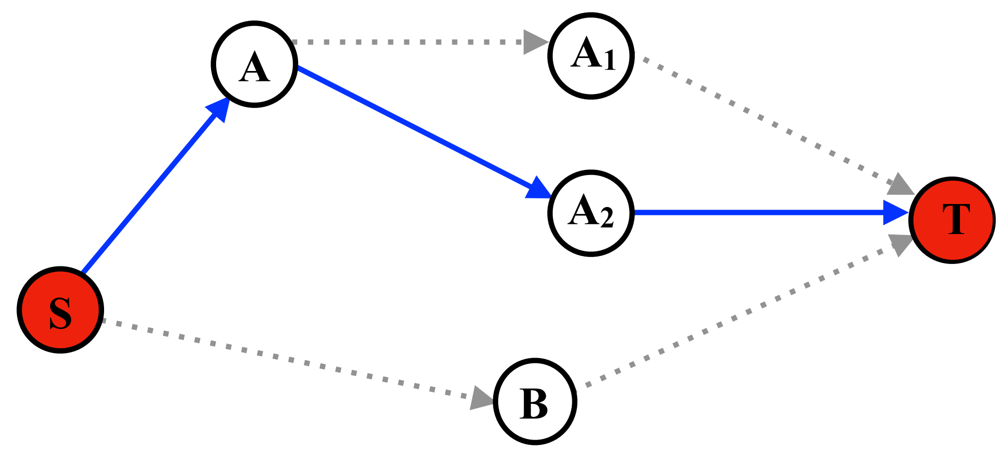
GDS: Graph with 6 nodes and 7 edges

S-I-R dynamics

property: vertices S and T are connected

x = probability of transmission through each edge





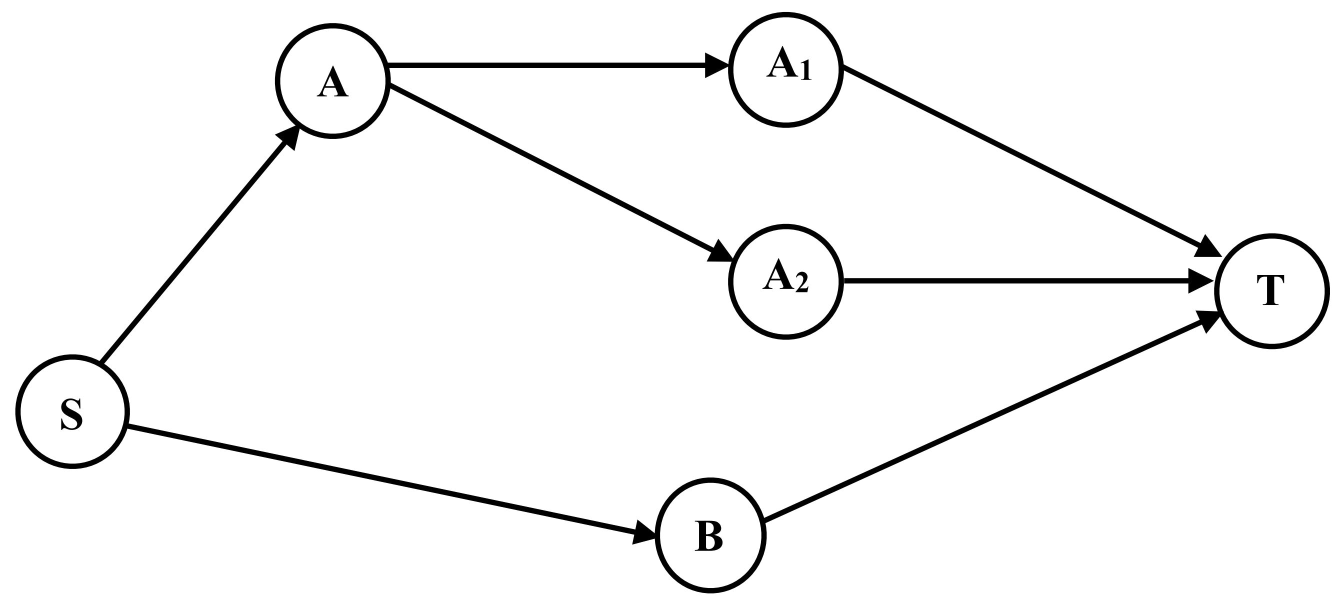
When these **three edges** are connected, S and T are connected

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Calculating network reliability for homogenous toy network (3/3)

Key Concepts

Assuming S is infected and others susceptible, what is the probability that T will be infected, i.e., probability that there exists a path between S and T?



GDS: Graph with 6 nodes and 7 edges

S-I-R dynamics

property: vertices S and T are connected

x = probability of transmission through each edge

$$
\begin{aligned}
&R(G, x) \\
&= x^2 + 2x^3 - 3x^5 + x^7 \\
&= \sum_{k=0}^{7} \alpha_k x^k, \quad \alpha_k = (0,0,1,2,0,-3,0,1) \\
&= \sum_{k=0}^{7} \beta_k \binom{7}{k} x^k (1-x)^{7-k}
\end{aligned}
$$

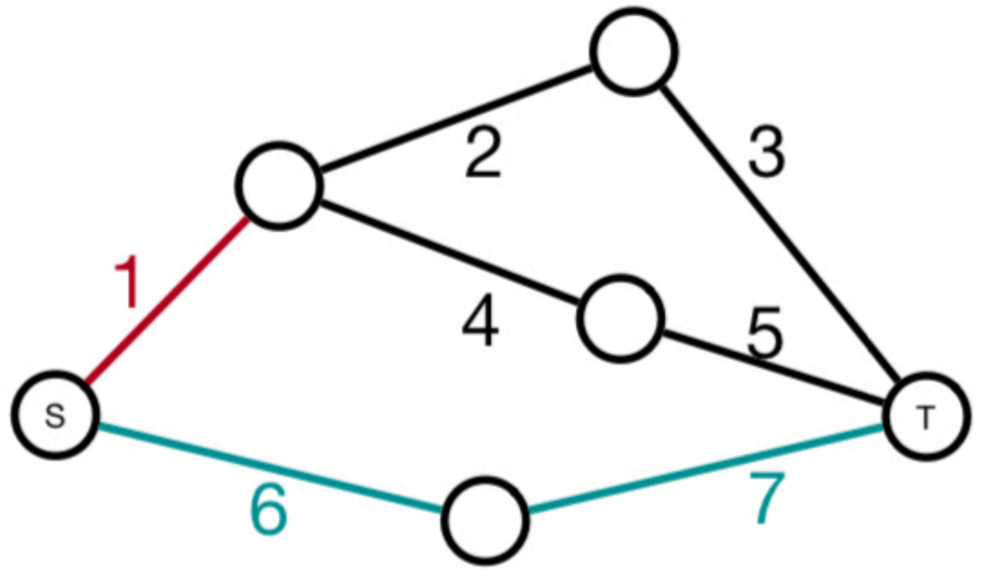
$$\beta_k = \left(0,0,\frac{1}{21},\frac{1}{5},\frac{18}{35},\frac{19}{21},1,1\right)$$

Using Inclusion-Exclusion principle

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

What is the probability that a path exists between two nodes S and T?

Key Concepts



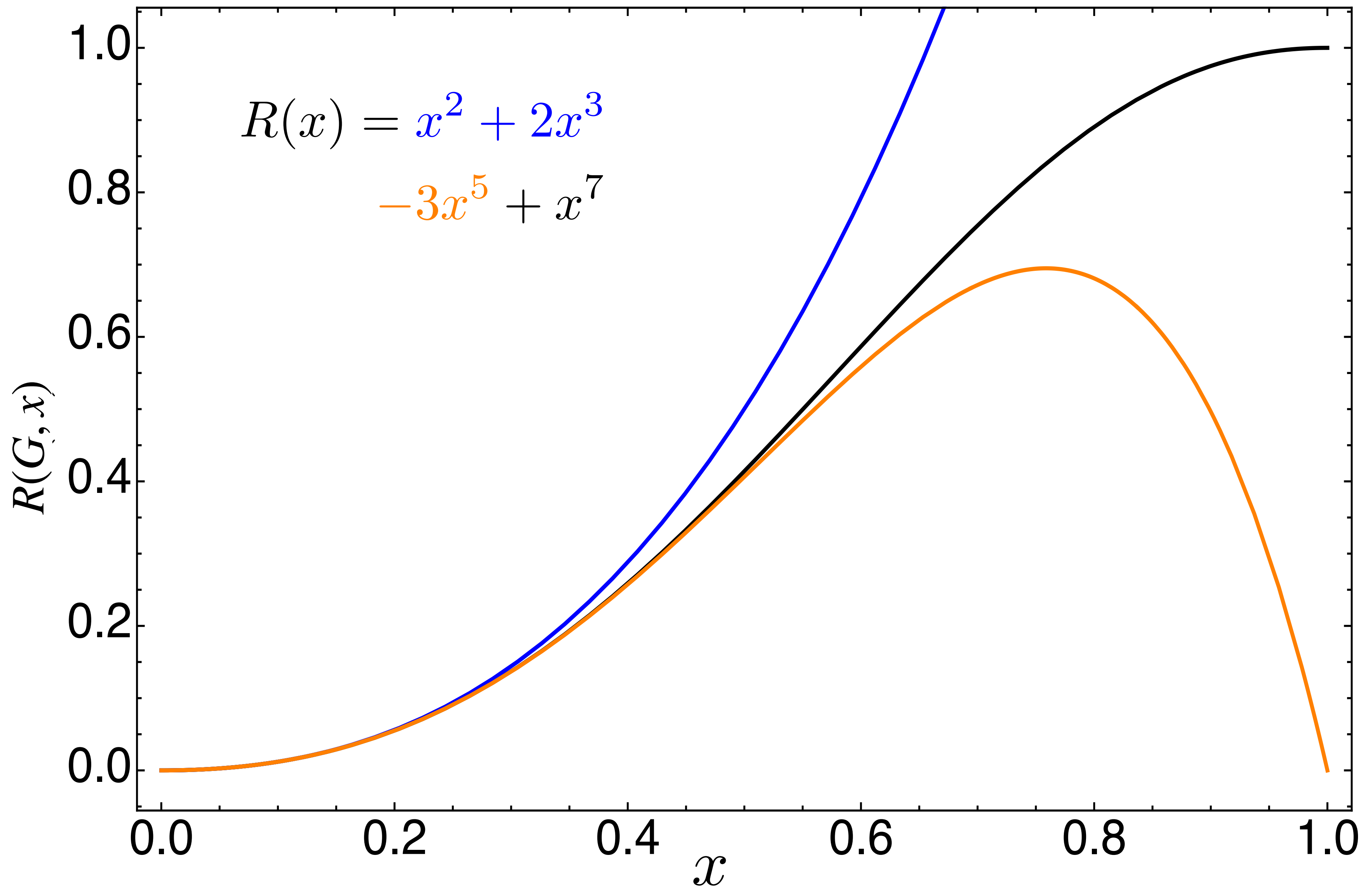
$$R(G,x) = x^2 + x^3 - 3x^5 + x^7$$

$$= \sum_{k=0}^{7} \alpha_k x^k$$

$$\alpha_k = (0,0,1,2,0,-3,0,1)$$

$$= \sum_{k=0}^{7} \beta_k \binom{7}{k} x^k (1-x)^{7-k}$$

$$\beta_k = \bar{\beta}_{7-k} = \left(0,0,\frac{1}{21},\frac{1}{5},\frac{18}{35},\frac{19}{21},1,1\right)$$



Taylor expansions around $x = 0 \rightarrow \sum_{k=0}^{N} \alpha_k x^k$

Eubank, S., et. al., Perturbative methods for mostly monotonic probabilistic satisfiability problems. arXiv preprint arXiv:2206.03550, 2022.

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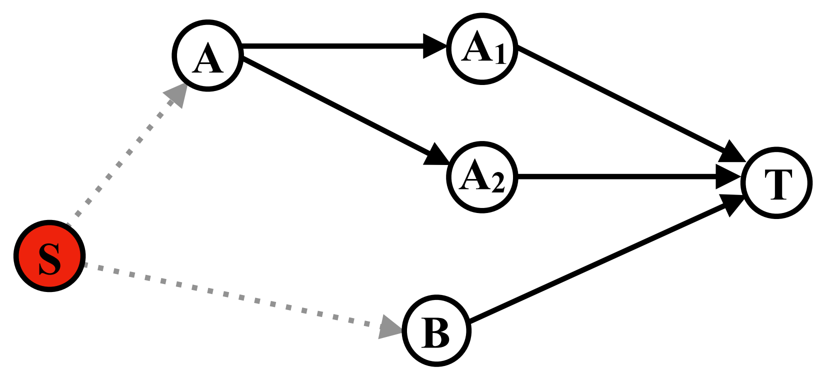
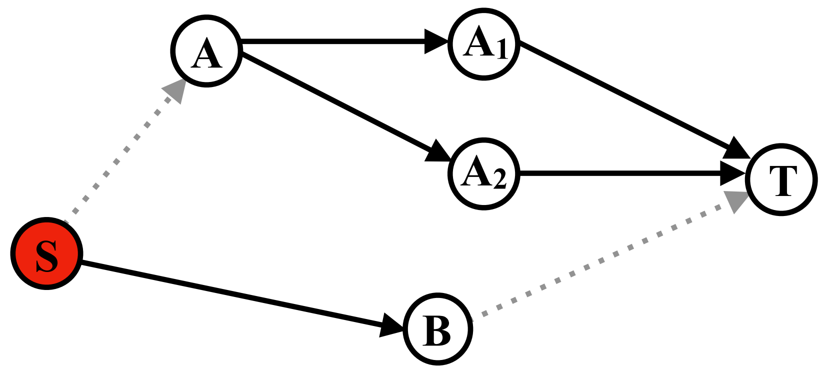
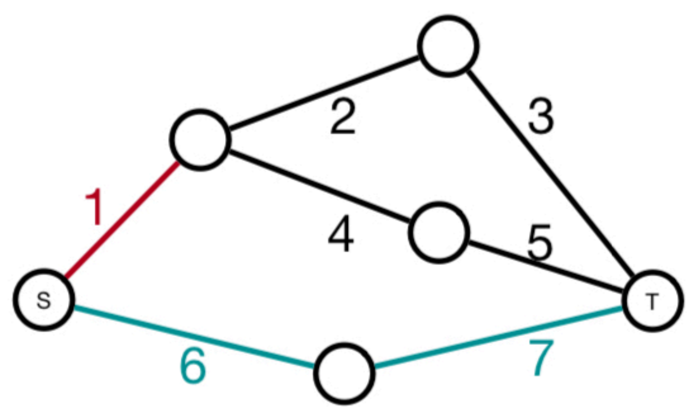
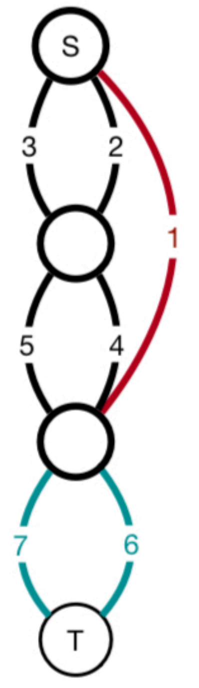
What is the probability that a path does not exist between two nodes S and T?

Key Concepts









At minimum, **removal of the two edges** - (1,6) or (1,7) are required for S and T not to be connected

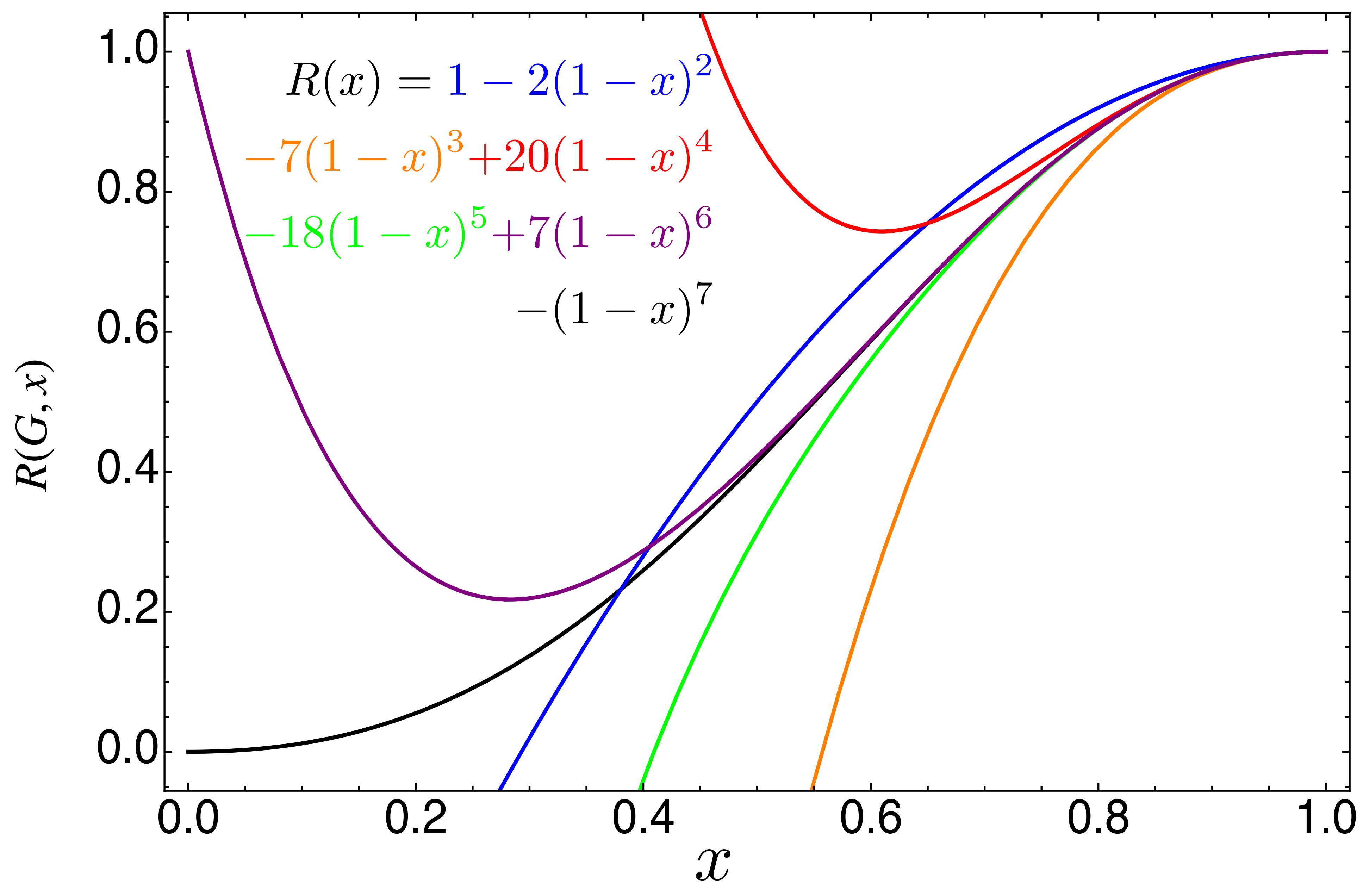
$$R(G,x) = x^2 + x^3 - 3x^5 + x^7$$

$$= \sum_{k=0}^{7} \overline{\alpha}_k (1-x)^k$$

$$\overline{\alpha}_k = (1,0,-2,-7,20,-18,7,-1)$$

$$= \sum_{k=0}^{7} \overline{\beta}_{7-k} \binom{7}{k} x^k (1-x)^{7-k}$$

$$\beta_k = \overline{\beta}_{7-k} = \left(0,0,\frac{1}{21},\frac{1}{5},\frac{18}{35},\frac{19}{21},1,1\right)$$



Taylor expansions around $x = 1 \rightarrow \sum_{k=0}^{N} \overline{\alpha}_k (1-x)^k$

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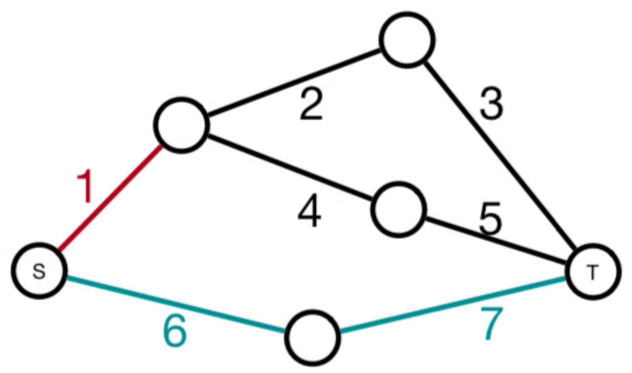

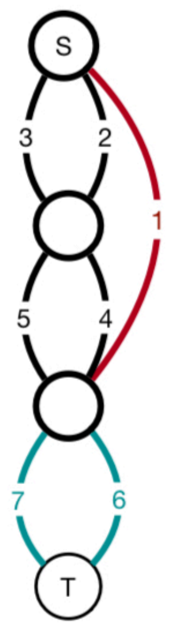

Why calculating “not connected” piece?

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Use it to calculate the reliability curve at the "end points"

Key Concepts

Recall:

$$
\begin{aligned}
R(G,x) &\equiv \text{network reliability} \\
&= 1 - \overline{R}(G, 1-x) \\
&= \sum_{k=0}^{N} \beta_k \binom{N}{k} x^k (1-x)^{N-k} \\
&= \sum_{k=0}^{N} \beta_k B(N,k,x) = \sum_{k=0}^{N} \alpha_k x^k \\
&= \sum_{k=0}^{N} \overline{\beta}_{N-k} B(N,k,x) = \sum_{k=0}^{N} \overline{\alpha}_k (1-x)^k
\end{aligned}
$$

$R(G, x)$ is the two-point correlation function in statistical physics.

Taylor expansions around $x = 0 \rightarrow \sum_{k=0}^{N} \alpha_k x^k$

$\Longrightarrow$ Weak-coupling expansion

Taylor expansions around $x = 1 \rightarrow \sum_{k=0}^{N} \overline{\alpha}_k (1-x)^k$

$\Longrightarrow$ Strong-coupling expansion

$\boxed{\text{Use perturbation approach to evaluate network reliability.}}$

Eubank, S., et. al., Perturbative methods for mostly monotonic probabilistic satisfiability problems. arXiv preprint arXiv:2206.03550, 2022.

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Problem!

The duality imposes constraints on the coefficients that are typically not respected by the Taylor expansions.

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Problem!

The duality imposes constraints on the coefficients that are typically not respected by the Taylor expansions.

Solution

Can be easily satisfied by transforming from power basis to Bernstein basis.

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Bernstein functions are useful to calculate network reliability

Key Concepts

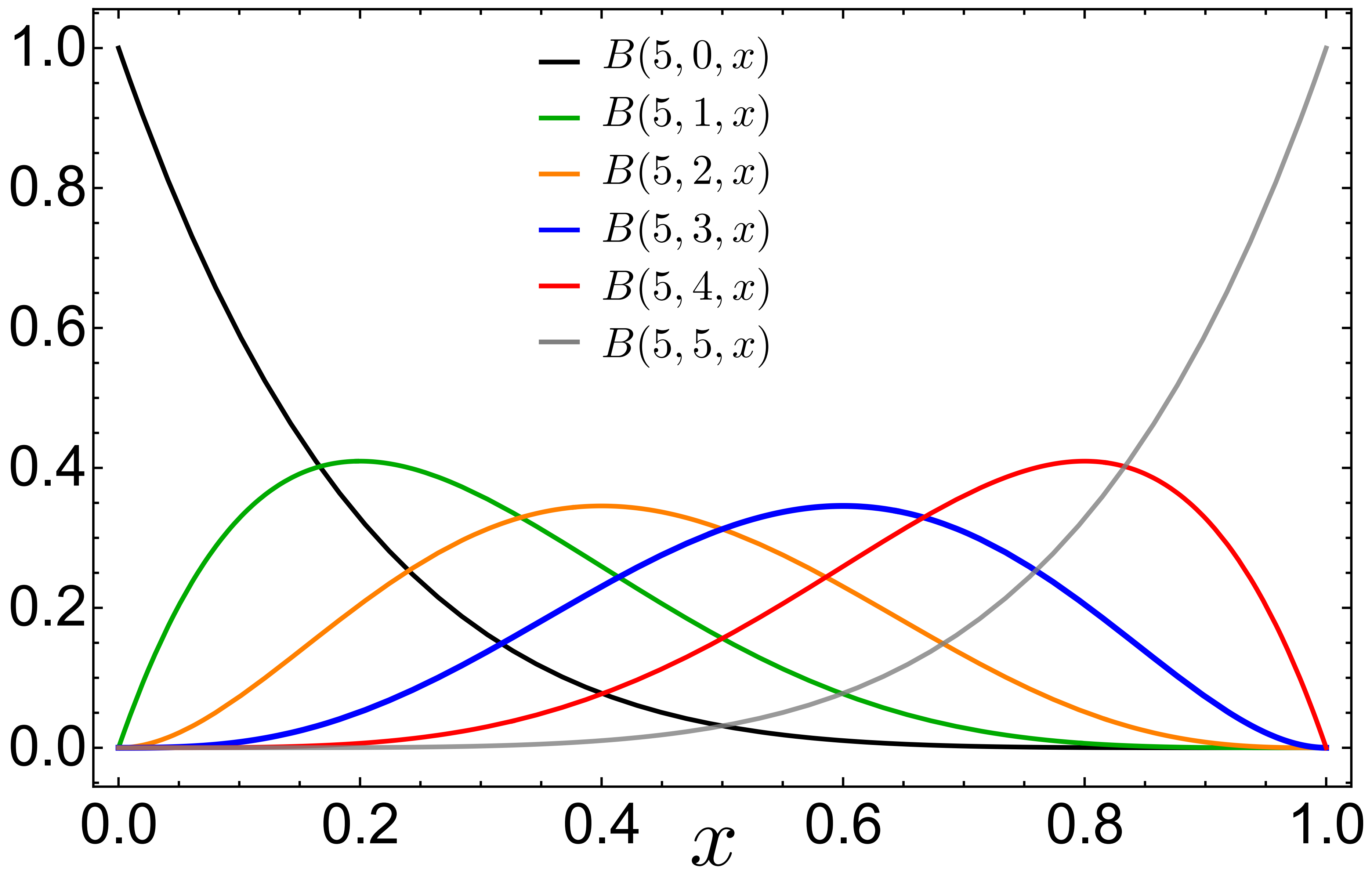
Bernstein basis function (natural basis for $R(G,x)$)

$$B(N,k,x) \equiv \binom{N}{k} x^k (1-x)^{N-k}$$

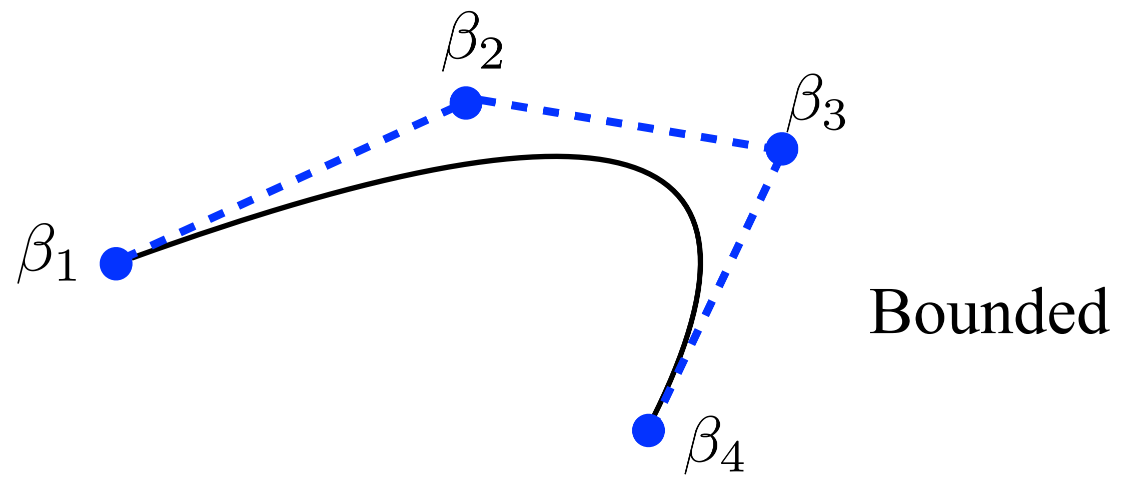
Duality property:

$$B(N,k,x) = B(N, N-k, 1-x)$$

$$\beta_k = \bar{\beta}_{N-k} = \text{Bezier/Bernstein coefficients}$$



$$\begin{aligned} R(G,x) &\equiv \text{network reliability} \\ &= 1 - \bar{R}(G, 1-x) \\ &= \sum_{k=0}^{N} \beta_k \binom{N}{k} x^k (1-x)^{N-k} \\ &= \sum_{k=0}^{N} \beta_k B(N,k,x) = \sum_{k=0}^{N} \bar{\beta}_{N-k} B(N,k,x) \end{aligned}$$



Lorentz, G.: Bernstein polynomials, American Mathematical Soc., 2012. Bernstein, S.: Comm. Soc. Math. Kharkov 13.1, 1912.

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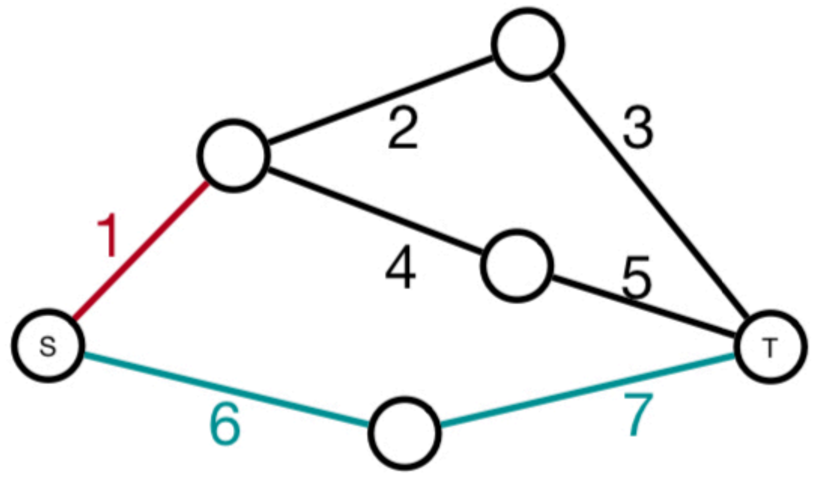
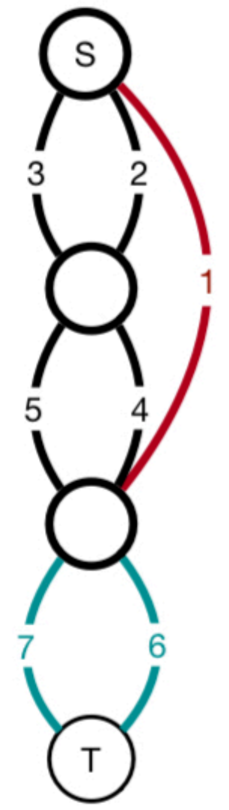
Perturbative methods provide sufficiently good estimates for network reliability (1/2)

Solution

What is the probability that a path exists between two nodes S and T?





GDS: Graph with 6 nodes and 7 edges

S-I-R dynamics

property: vertices S and T are connected

x = probability of transmission through each edge

Let's consider

- terms up to $O(x^3)$ for $R(G,x)$, i.e., at $x=0$,
- terms up to $O((1-x)^2)$ for $\overline{R}(G,x)$, i.e., at $x=1$

$$R(G,x)$$

$$= \sum_{k=0}^{7} \alpha_k x^k = \sum_{k=0}^{7} \overline{\alpha}_k (1-x)^k$$

known $\alpha_k = (0,0,1,2)$

known $\overline{\alpha}_k = (1,0,-2)$

$$= \sum_{k=0}^{7} \beta_k B(7,k,x)$$

$$\beta_k = \overline{\beta}_{7-k} = \left(0,0,\frac{1}{21},\frac{1}{5},\text{unknown},\text{unknown},1,1\right)$$

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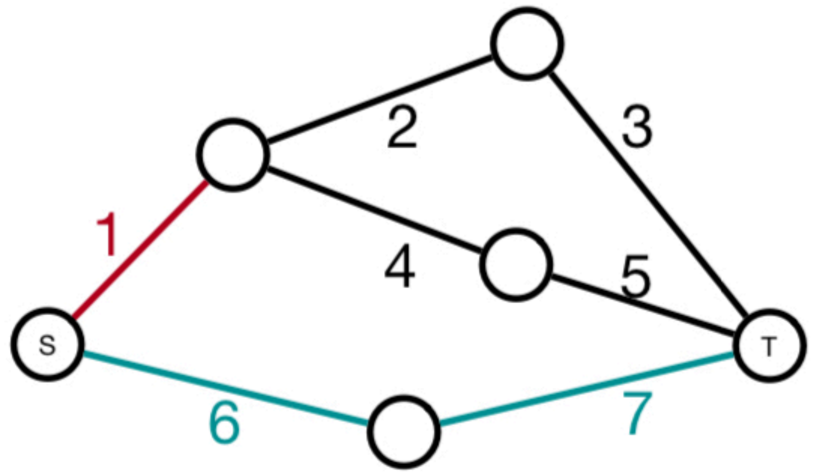
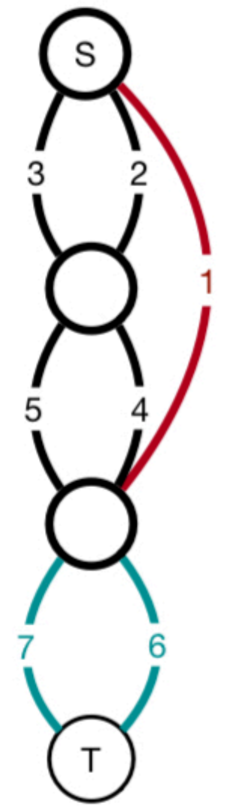
Perturbative methods provide sufficiently good estimates for network reliability (2/2)

Solution

What is the probability that a path exists between two nodes S and T?



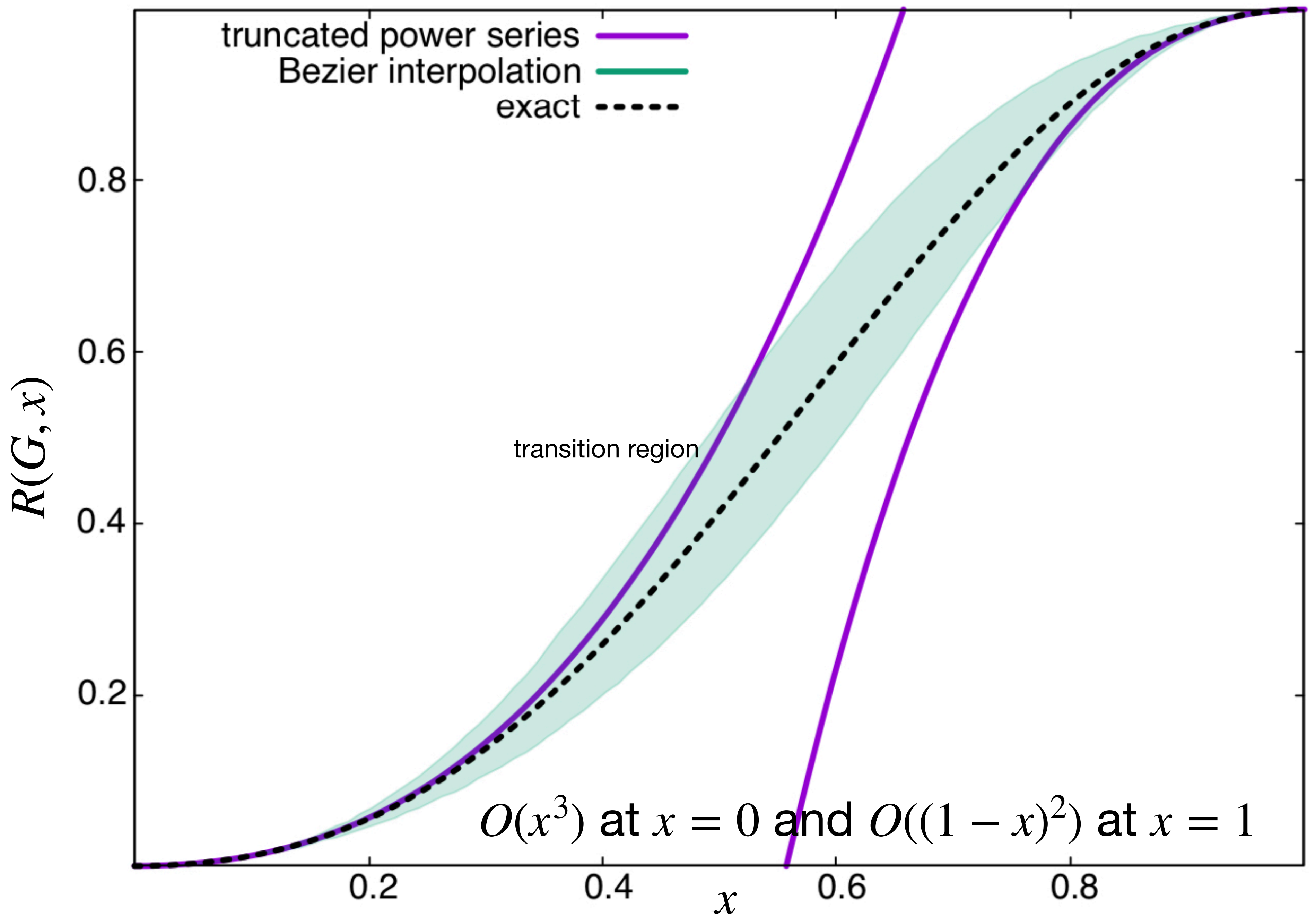


GDS: Graph with 6 nodes and 7 edges

S-I-R dynamics

property: vertices S and T are connected

x = probability of transmission through each edge



Eubank, S., et. al., Perturbative methods for mostly monotonic probabilistic satisfiability problems. arXiv preprint arXiv:2206.03550, 2022.

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

The exact evaluation of all network reliability polynomials for these diffusive processes is a #P-hard problem

Key Concepts

For larger networks Monte Carlo simulations are required

Monte-Carlo simulations can evaluate precise estimates of coefficients for larger networks. Each simulation run provides one sample of a Bernoulli process.

However, Monte-Carlo simulations are not efficient in the limits when small number of sites satisfy the property, i.e., they perform well only at the "middle region".

- Monte-Carlo succeeds when $k \sim \frac{N}{2}$, i.e., k is large

- Monte-Carlo not efficient when $k \ll N$, i.e., k is small

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Combination of perturbative methods and Monte-Carlo simulations provide better estimations of reliability on real-world directed, weighted networks

Solution

Recall:

$R(G, x) \equiv$ network reliability

$$= \sum_{k=0}^{N} \beta_k \binom{N}{k} x^k (1-x)^{N-k}$$

$$= \sum_{k=0}^{N} \beta_k B(N,k,x) = \sum_{k=0}^{N} \alpha_k x^k$$

$$= \sum_{k=0}^{N} \bar{\beta}_{N-k} B(N,k,x) = \sum_{k=0}^{N} \bar{\alpha}_k (1-x)^k$$

$$= 1 - \bar{R}(G, 1-x)$$

$$B(N,k,x) \equiv \binom{N}{k} x^k (1-x)^{N-k}$$

Bernstein basis function

$\beta_k = \bar{\beta}_{N-k} \rightarrow$ Bezier/Bernstein coefficients

$\alpha_k, \bar{\alpha}_k \rightarrow$ Taylor series coefficients

<u>For efficient estimation and interpolation</u>:

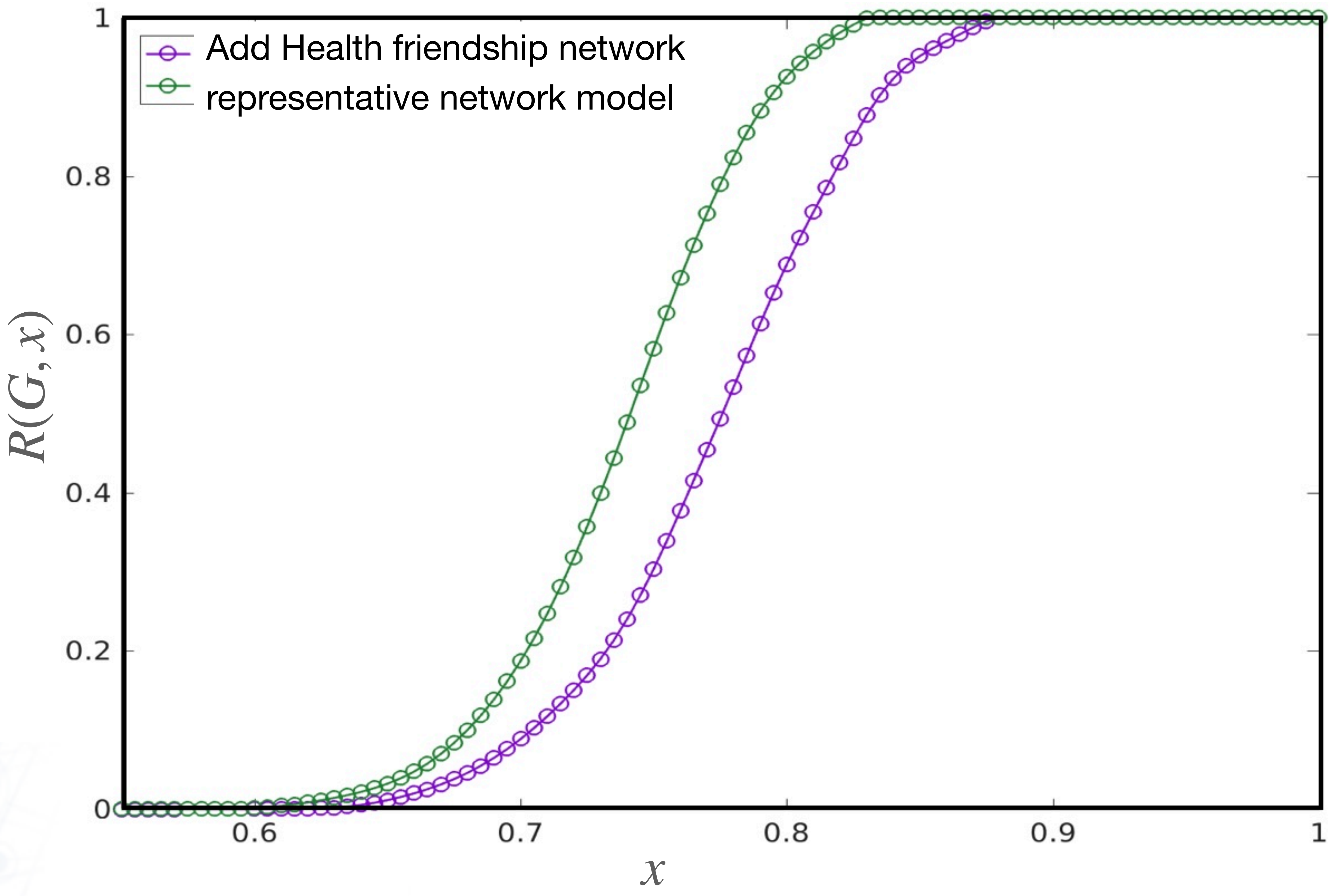
1. Perturbative expansions of $R(G, x)$ around $x = 0$ and $1 - \bar{R}(G, 1-x)$ around $x = 1$ are given by the Inclusion/Exclusion expansions.
2. The duality imposes constraints on the coefficients that are typically not respected by the Taylor expansions, but can be easily satisfied by transforming from power basis to Bernstein basis.
3. Interpolate between the "two ends". For better results, add Monte-Carlo estimates for the "middle portion".

Eubank, S., et. al., Perturbative methods for mostly monotonic probabilistic satisfiability problems. arXiv preprint arXiv:2206.03550, 2022.

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Reliability curves to estimate epidemic outbreak on susceptible population

Given a network of susceptible population, network reliability is the probability that a certain fraction of the population is infected from a random infected node in an SIR process when the probability of transmission of infection is x.



Reliability curves

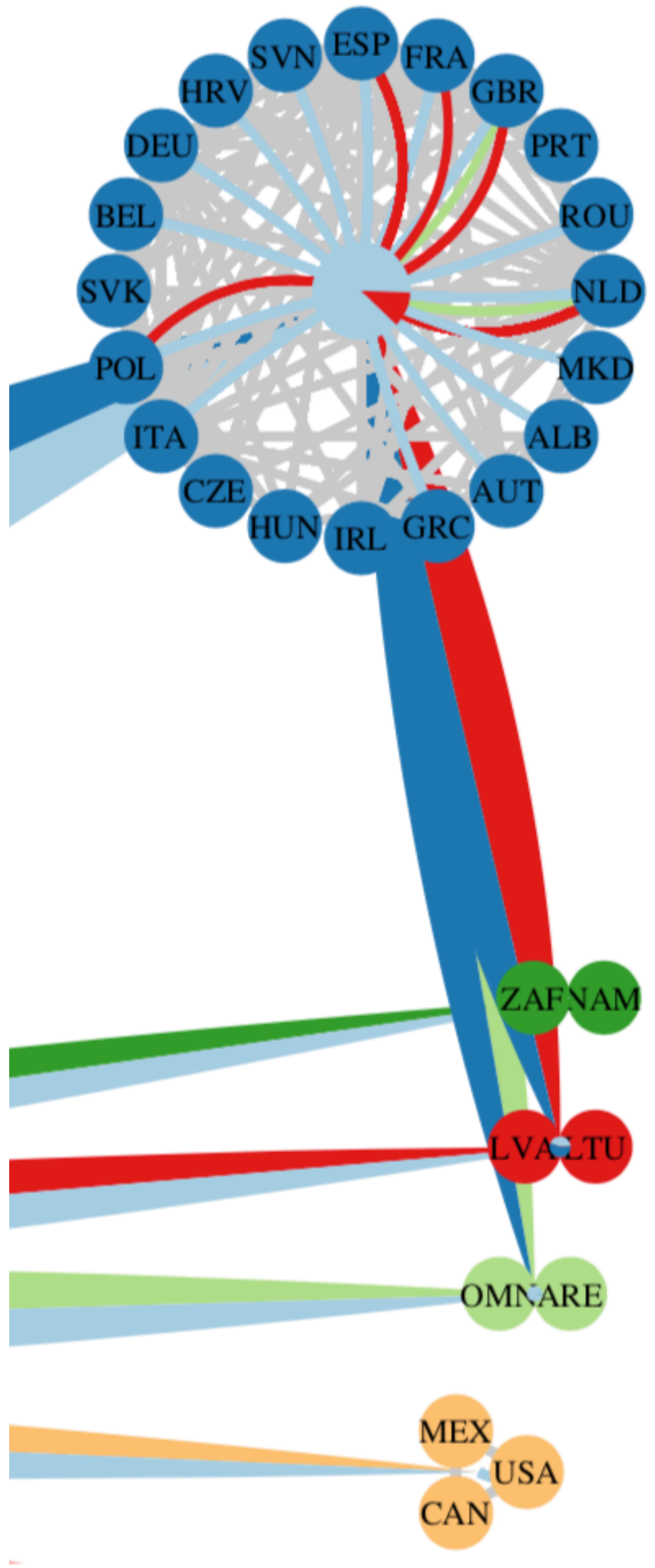
- estimate epidemic potential on networks
- determine consistency of the results between two networks

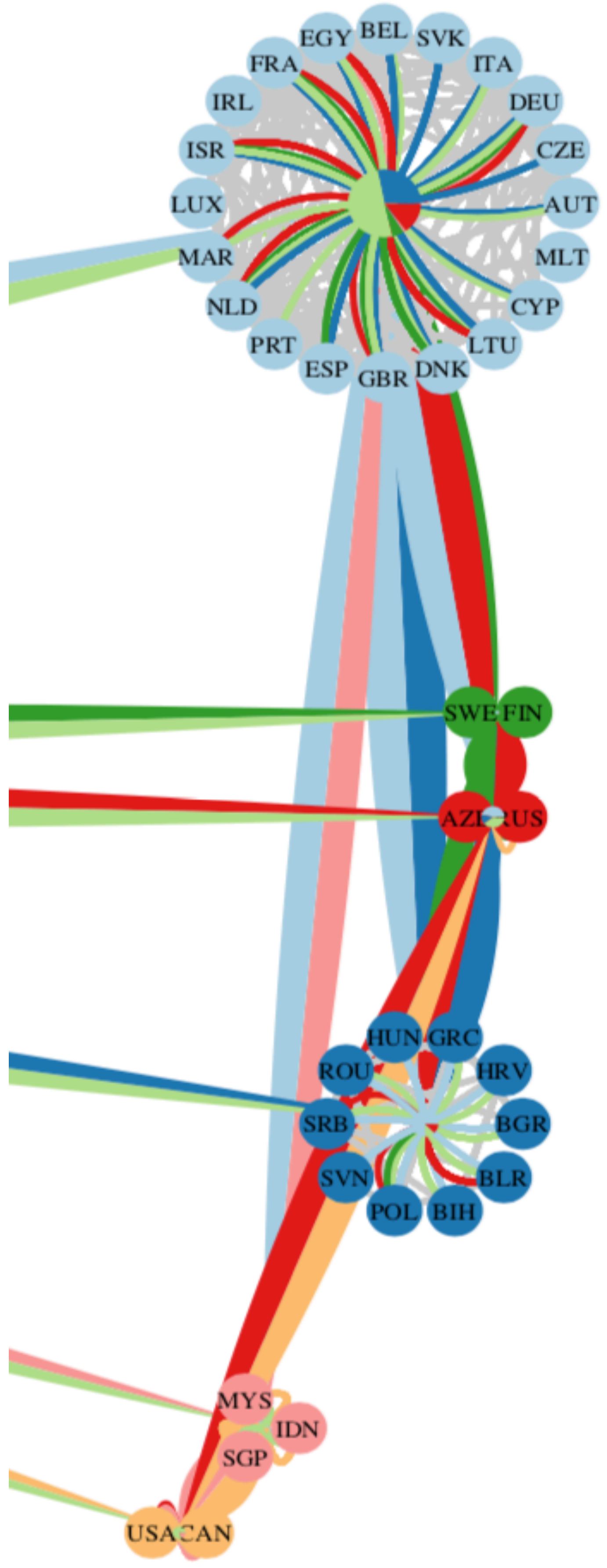
Nath, M., et al. Determining whether a class of random graphs is consistent with an observed contact network. Journal of theoretical biology 440 (2018): 121-132.

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Reliability identifies strongly connected clusters of vulnerable countries from international food trade networks

Given a network of international food trade patterns, network reliability gives clusters of strongly connected countries of certain size. The probability of infecting the countries inside such a cluster is higher when any one of these countries is affected by the pest.





Labels indicate country names (ISO code).

Clusters identified indicate that
- concur with the world trade agreements and distinguish between types of commodities
- tomato tomato - regional trade
- potato (staple crop) - global trade

(Tomato & Potato: Hosts for pest *Tuta absoluta*)

Nath, M., et.al.,: Using Network Reliability to Understand International Food Trade Dynamics, Proceedings of The Conference on Complex Networks 2018.

Nath, M., Application of Network Reliability to Analyze Diffusive Processes on Graph Dynamical Systems, 2019.

Newton’s scientific method

“By this way of **Analysis** we may proceed from Compounds to Ingredients, and from Motions to the Forces producing them; and in general, **from Effects to their Causes**, and from a particular Cause to more general ones, till the **Argument end in the most general**. This is the Method of Analysis: and the Synthesis consists in assuming the Causes discover’d, and establish’d as Principles, and by them **explaining the Phaenomena** proceeding from them, and proving the Explanations.”

— Isaac Newton, Opticks, Query 31, London, 3rd edition (1718)

Models - represent microscopic causes or macroscopic phenomenon.

Synthesis - connects macroscopic behaviour to the microscopic model.

Summary

"Realistic scenarios lie between perfect randomness and perfect order." - Z. Adam

Graph Dynamical System

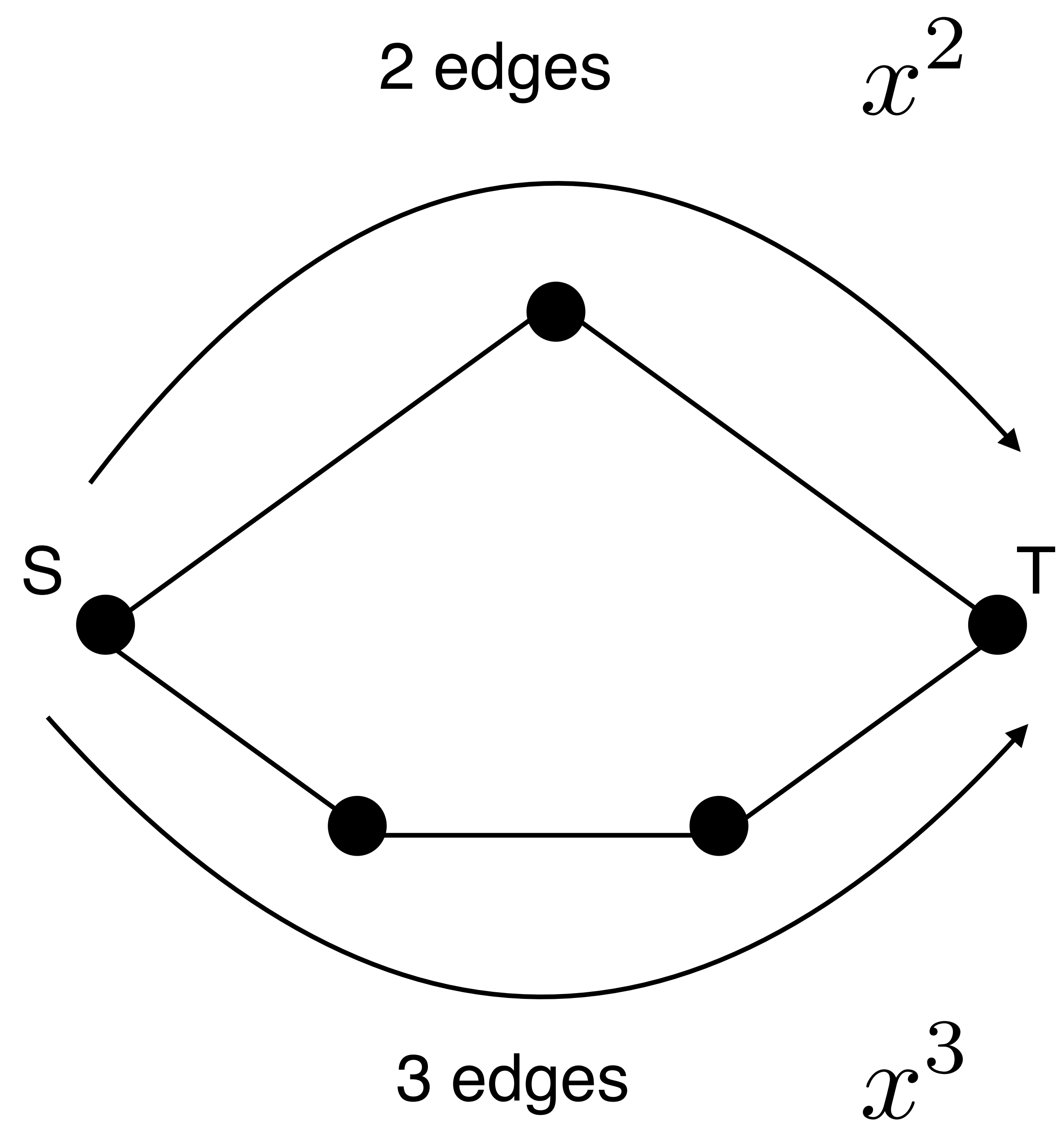
- provides a formal model to capture the structure and the dynamics,
- represent any system of discrete nodes whose state changes according to their interactions with neighbours.

Network reliability

- probability that a finite sized graph dynamical system in a specific configuration now will have a certain property later
- function of both structural and dynamical aspects of any system
- a generic tool with a wide range of applications
- can provide a new perspective on some old problems

APPENDIX

Inclusion-Exclusion Principle



Counting technique which generalizes the familiar method of obtaining the number of elements in the union of two finite sets

$$|A \cup B| = |A| + |B| - |A \cap B|$$

$$p(S \to T) = x^2 + x^3 - x^5$$

Bezier coefficients and Bezier curves

Appendix