Fast and Deterministic Computation of Fixation Probability in Evolutionary Graphs

Paulo Shakarian
Dept. Elec. Eng. and Computer Science
U.S. Military Academy, West Point

Patrick Roos
Dept. of Computer Science
University of Maryland, College Park

Network Science Center
West Point

Evolutionary Graph Theory

- How does population structure affect evolutionary dynamics?
  - E. Lieberman, C. Hauert, M. Nowak, “Evolutionary dynamics on graphs,” Nature 433:312–316 (2005)
  - Biological and Social Applications

Population:

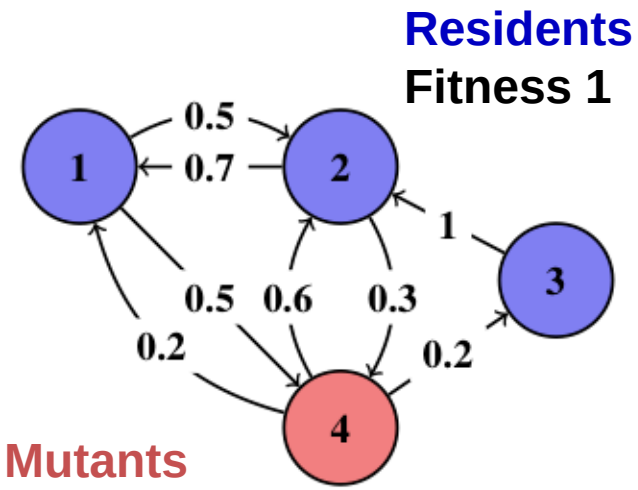
Structured on Graph

Nodes:

Individuals with Fitness

Edges:

Replacement Interactions



Fitness r (r=1 is “neutral drift”)

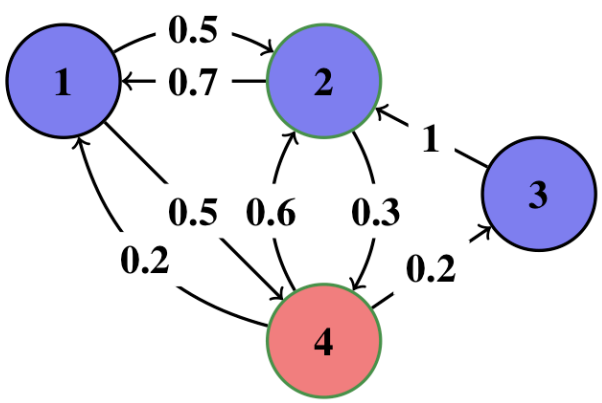
University of Maryland 1856
Network Science Center West Point

Moran Process (on Graphs)

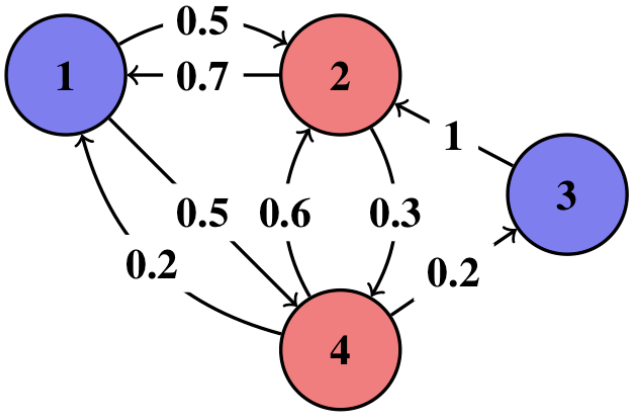
- Simple stochastic model to study selection in a finite population

- "Birth-Death" - At each time step:
  1. Choose an individual **I** for reproduction with a probability proportional to its fitness
  2. Random neighbor of **I** eliminated
  3. Offspring of **I** replaces eliminated neighbor

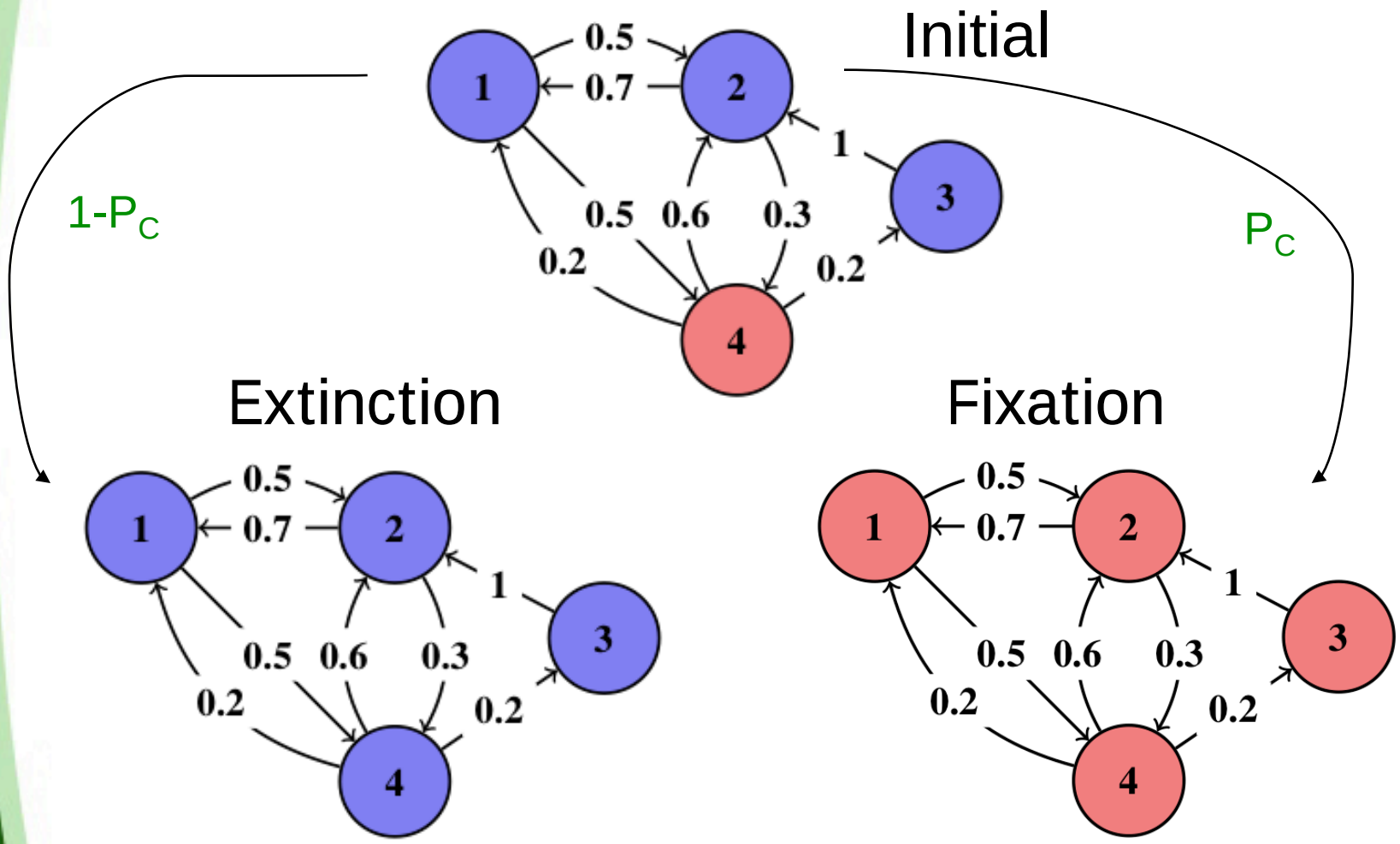
t = 1



t = 2



Two Absorbing States



Network Science Center
West Point

Fixation Probability

- The probability of a mutant invader overtaking a population

Basic Problem:

Given Mutant Node, Calculate Fixation Probability P_C

- Existing approaches for directed graphs rely on Monte Carlo Simulation, drawbacks:
  - Non-deterministic
  - Standard error can only be estimated
  - To ensure low standard error Monte Carlo simulation requires many runs – time consuming to compute
- We Provide Deterministic Fixation Probability Algorithm for strongly connected graphs

Theoretical Results

Vertex Probability: $\boldsymbol{Pr(M_i^{(t)})}$ is the probability that vertex $\boldsymbol{v_i}$ is a mutant at time $\boldsymbol{t}$.

Theorem 1. *If the graph is strongly connected,* $\forall i$, $lim_{t\to\infty} \boldsymbol{Pr}(\boldsymbol{M}_i^{(t)}) = P_C$.

Corollary 1. *Under* $r = 1$, $\boldsymbol{Pr}(\boldsymbol{M}_i^{(t)})$ *equals*

$$\frac{1}{N} \sum_{(v_j, v_i) \in E} w_{ji} \cdot \left(\boldsymbol{Pr}(\boldsymbol{M}_j^{(t-1)}) - \boldsymbol{Pr}(\boldsymbol{M}_i^{(t-1)}) \right) + \boldsymbol{Pr}(\boldsymbol{M}_i^{(t-1)})$$

Theorem 3. *When* $r = 1$, *if for some time* t, $\forall i$, *the value* $\boldsymbol{Pr}(\boldsymbol{M}_i^{(t)})$ *is the same, then* $\boldsymbol{Pr}(\boldsymbol{M}_i^{(t)}) = P_C$.

DFP (Deterministic Fixation Probability) Algorithm

Input: Evolutionary Graph $\langle N, V, W \rangle$, configuration $C \subseteq V$, natural number $R > 0$, and real number $\epsilon \geq 0$.
Output: Estimate of fixation probability of mutant.

---

p_i is the ith position in vector p corresponding with vertex $v_i \in V$.
Set $p_i = 1$ if $v_i \in C$ and $p_i = 0$ otherwise.
$\mathbf{q} \leftarrow \mathbf{p}$ {$\mathbf{q}$ will be $\mathbf{p}$ from the previous time step.}
$\tau \leftarrow 1$
while $\tau > \epsilon$ **do**
  for $v_i \in V$ **do**
    $sum \leftarrow 0$
    $\mathbf{m} \leftarrow \{v_j \in V | w_{ji} > 0\}$
    for $v_j \in m$ **do**
      $sum = sum + w_{ji} \cdot (\mathbf{q}_j - \mathbf{q}_i)$
    end for
    $\mathbf{p}_i \leftarrow \mathbf{q}_i + 1/N \cdot sum$
  end for
  $\mathbf{q} \leftarrow \mathbf{p}$
  $\tau \leftarrow (1/2) \cdot (\max p - \min p)$
end while
return $(\min p) + \tau$

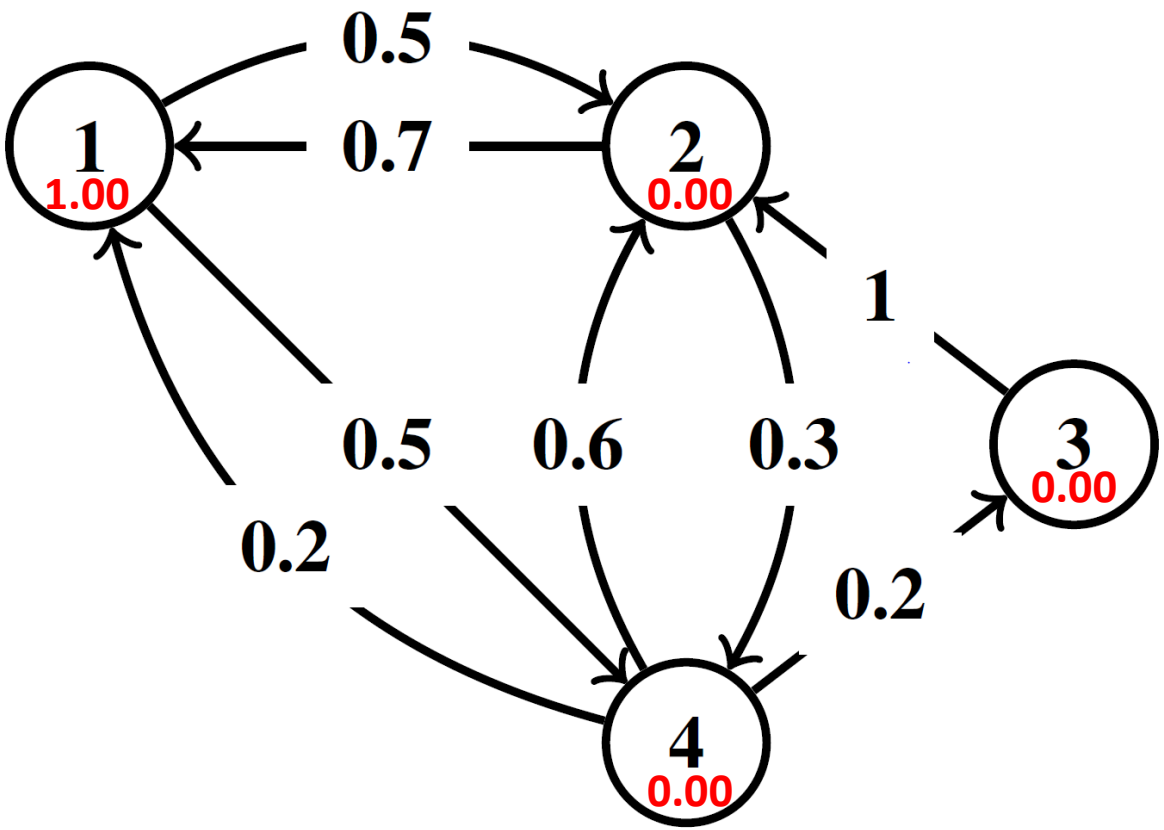
Vertex probability vectors at t and t-1

Until vertex probabilities have converged enough

Update vertex probabilities according to summation over neighbors.

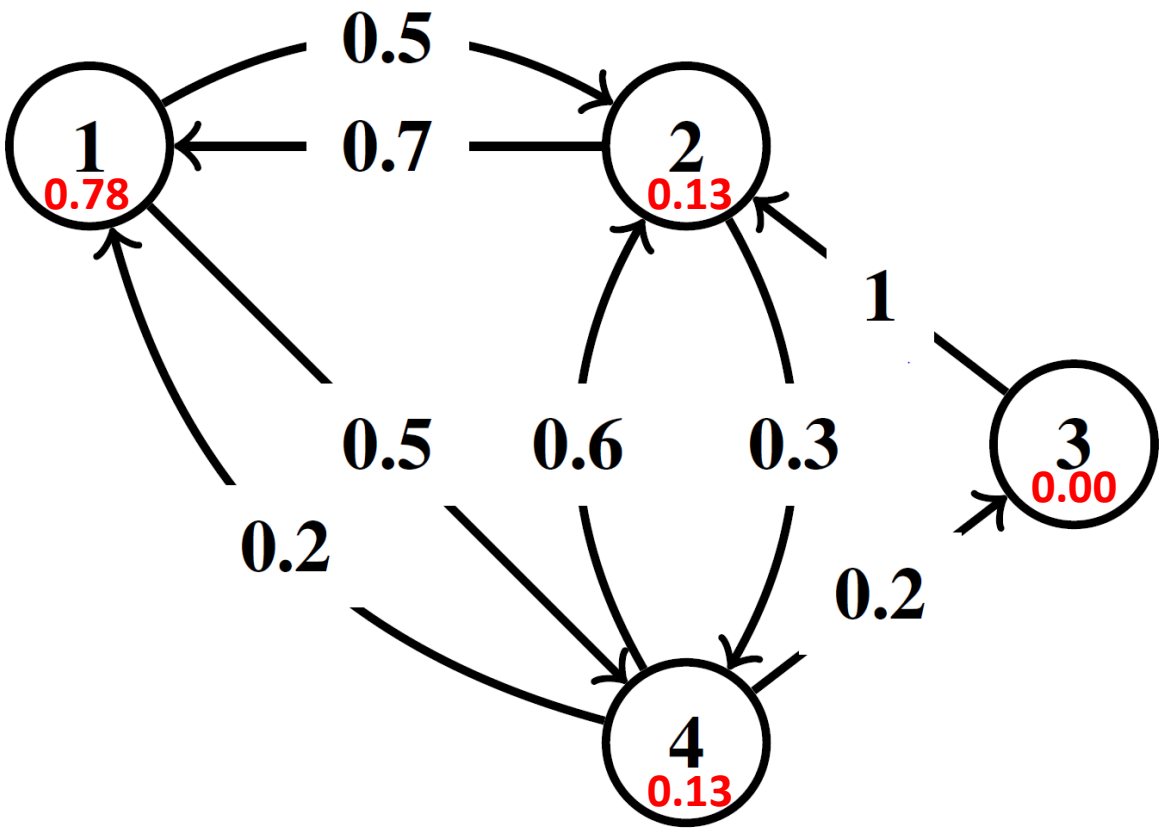
UNIVERSITY OF MARYLAND 1856
nce Center
West Point

Initial



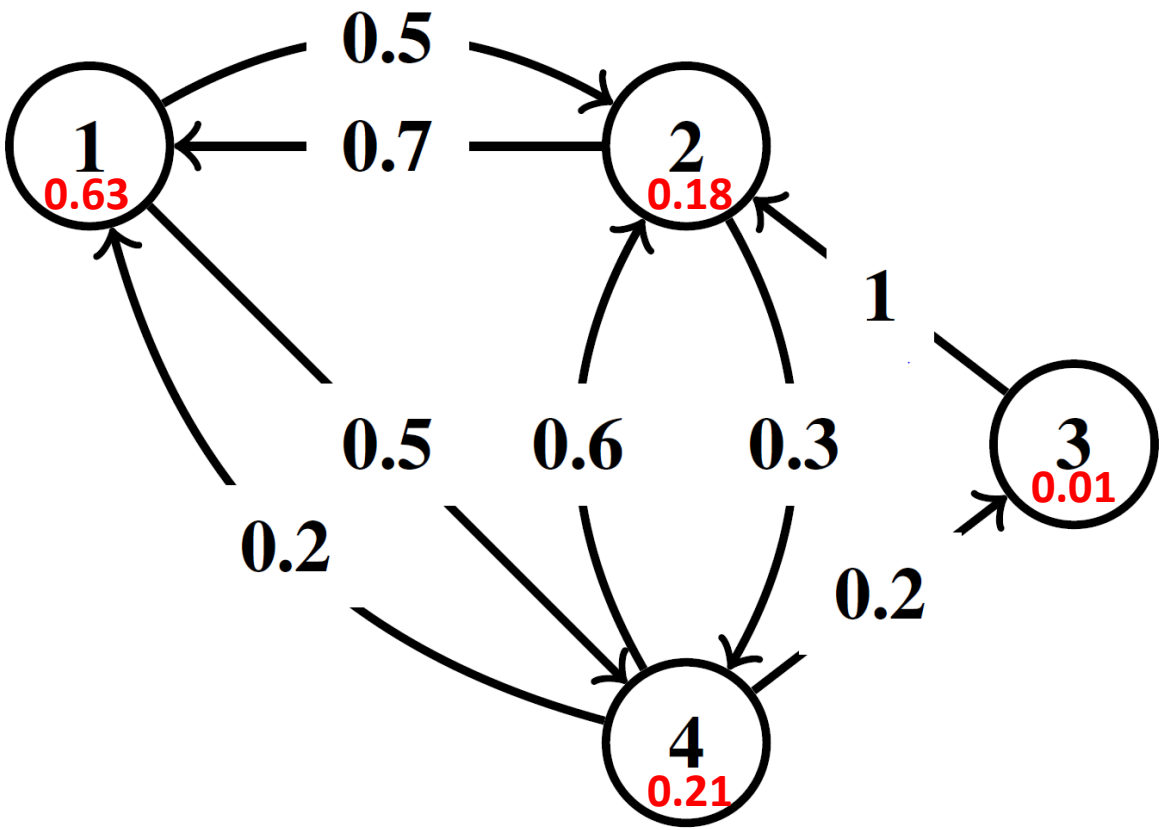
UNIVERSITY OF MARYLAND 1856
Network Science Center
West Point

After 1 Iteration



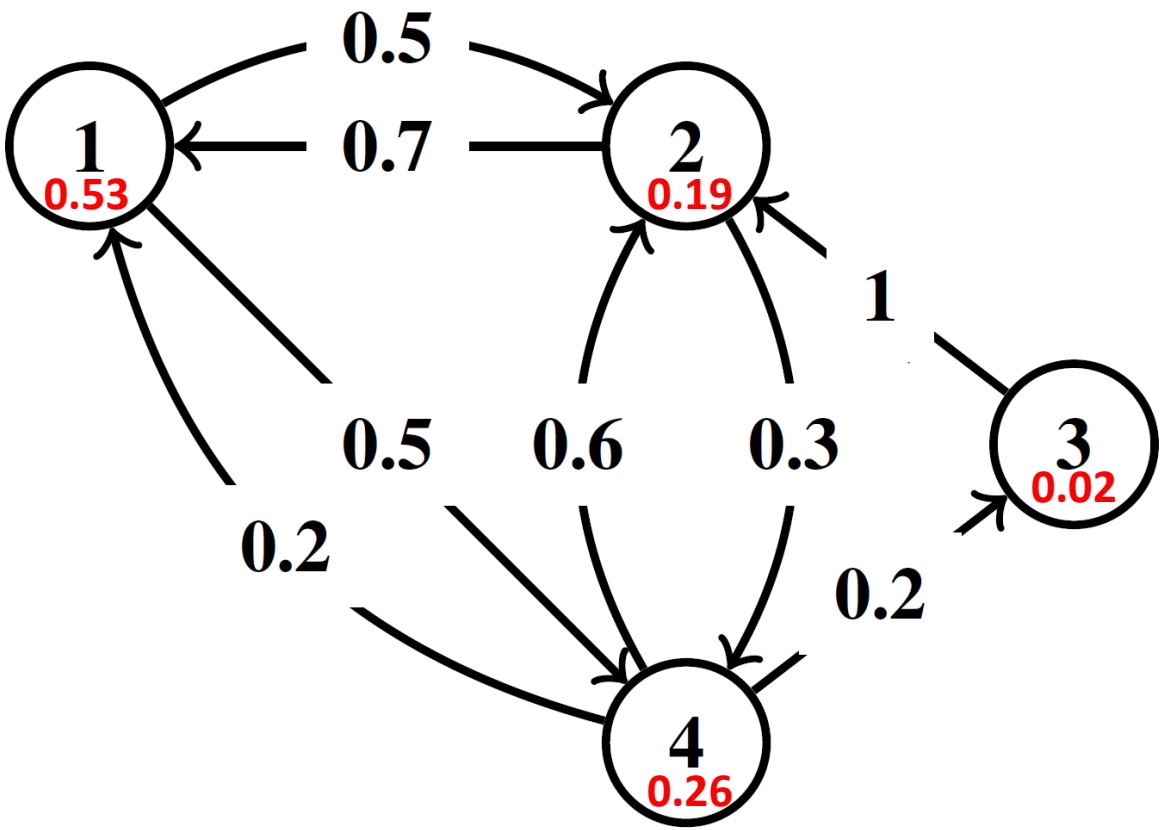
Network Science Center
West Point

After 2 Iterations



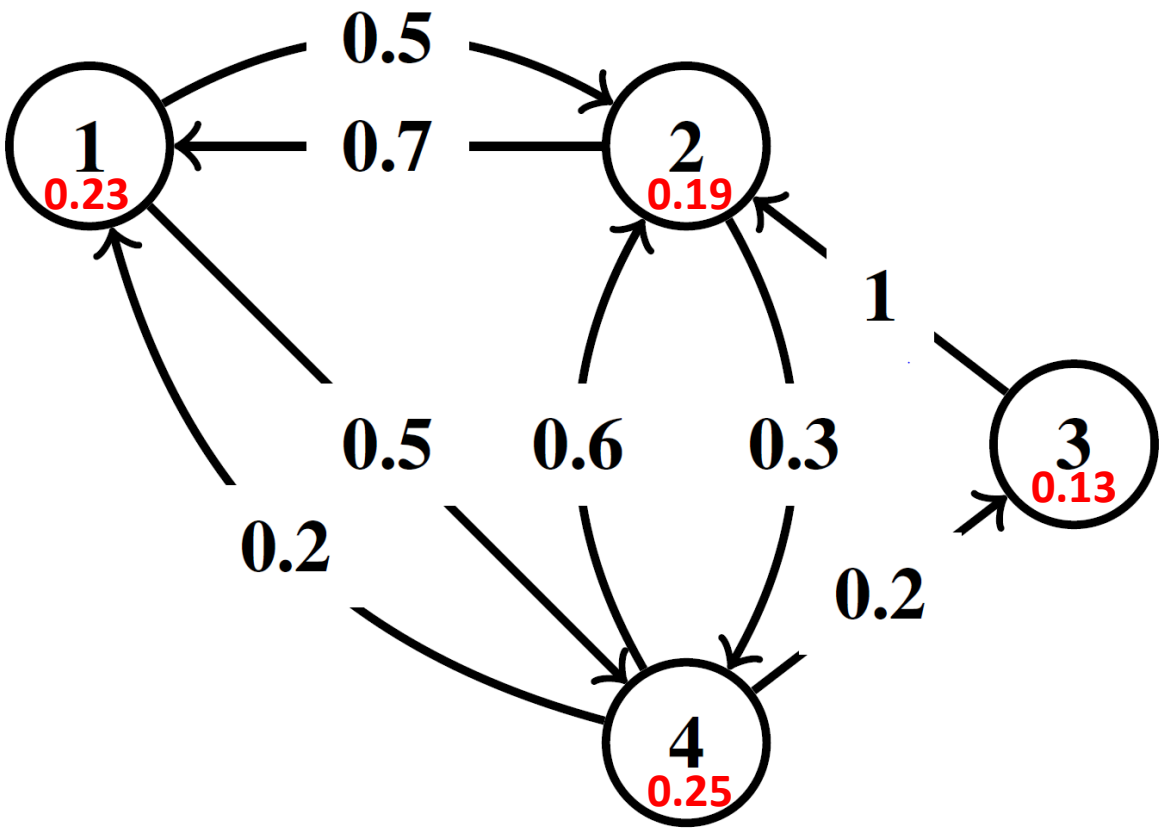
UNIVERSITY OF MARYLAND 1856
Network Science Center
West Point

After 3 Iterations



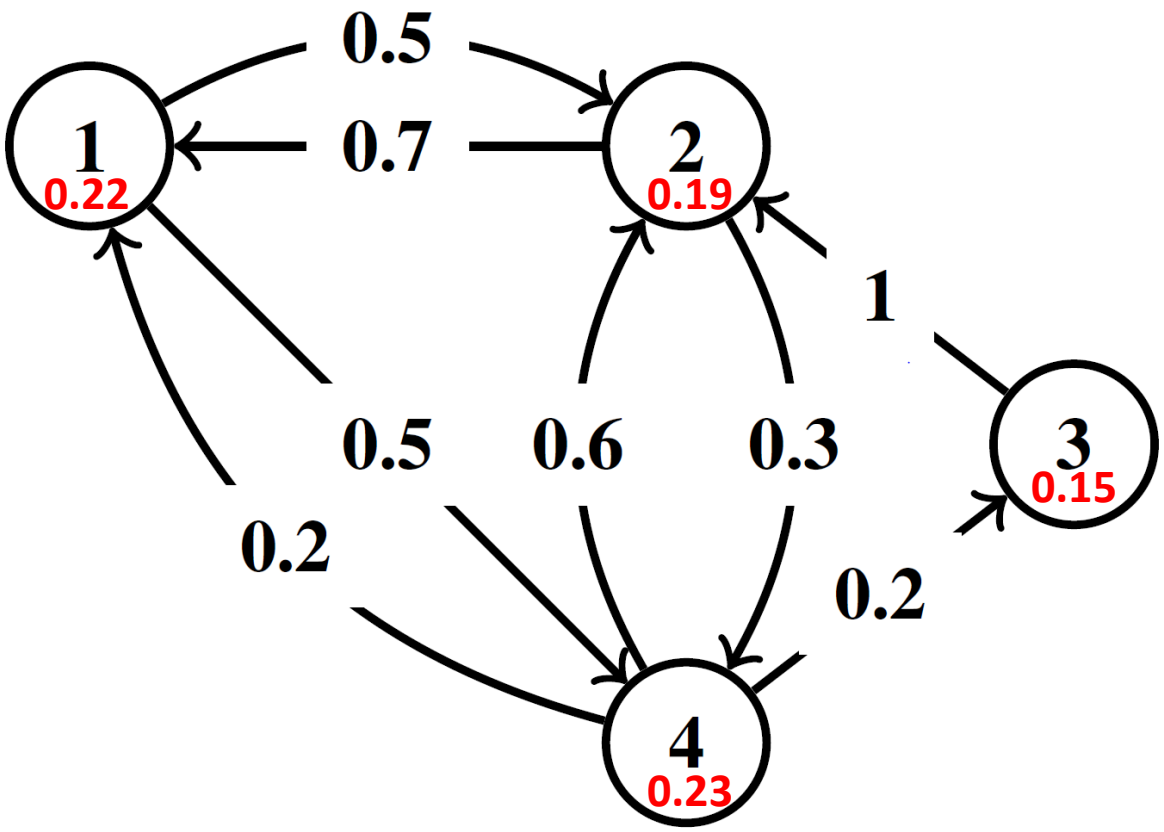
UNIVERSITY OF MARYLAND 1856
Network Science Center
West Point

After 14 Iterations



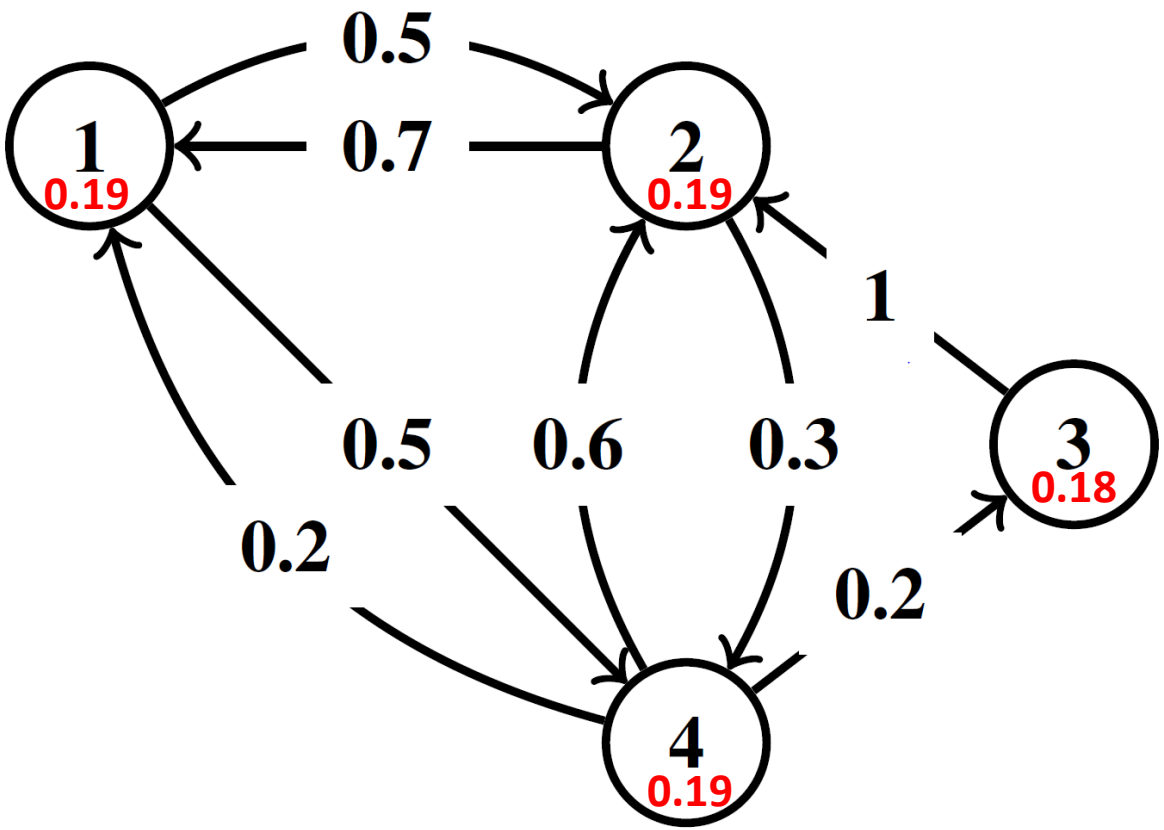
UNIVERSITY OF MARYLAND 1856
Network Science Center
West Point

After 17 Iterations



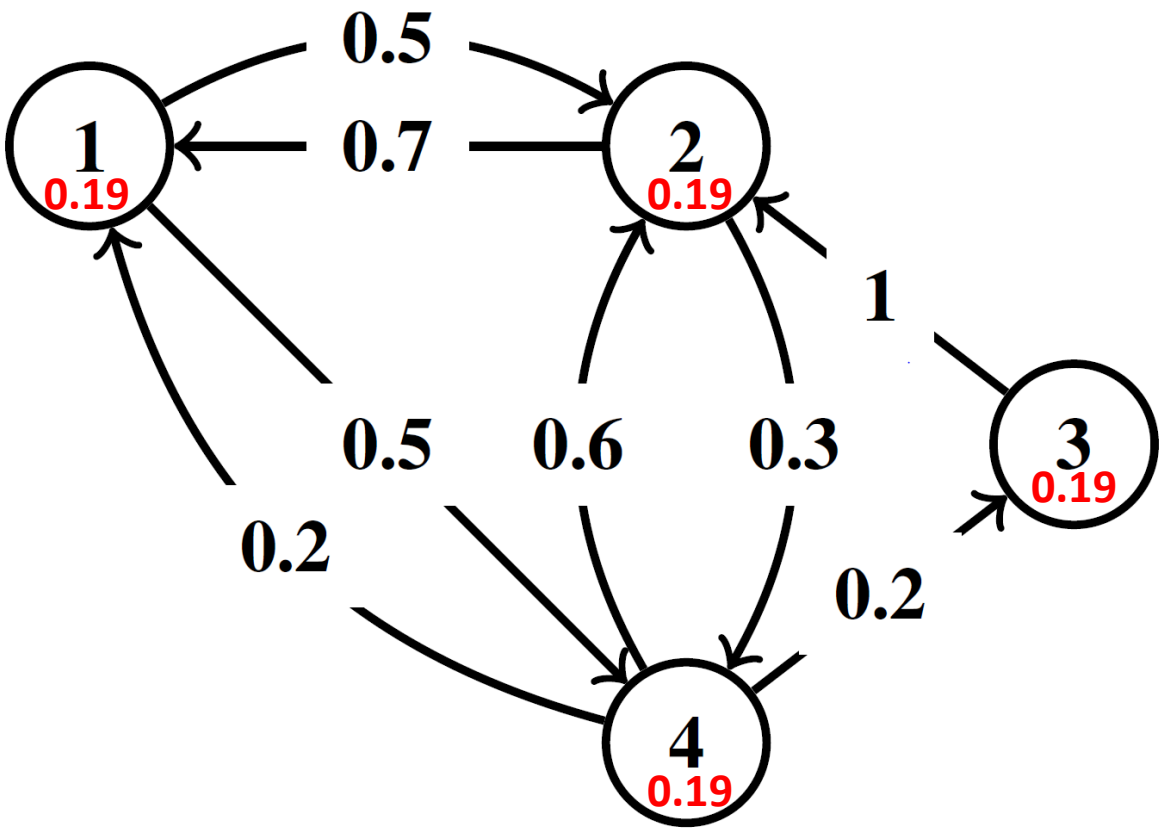
UNIVERSITY OF MARYLAND 1856
Network Science Center
West Point

After 50 Iterations



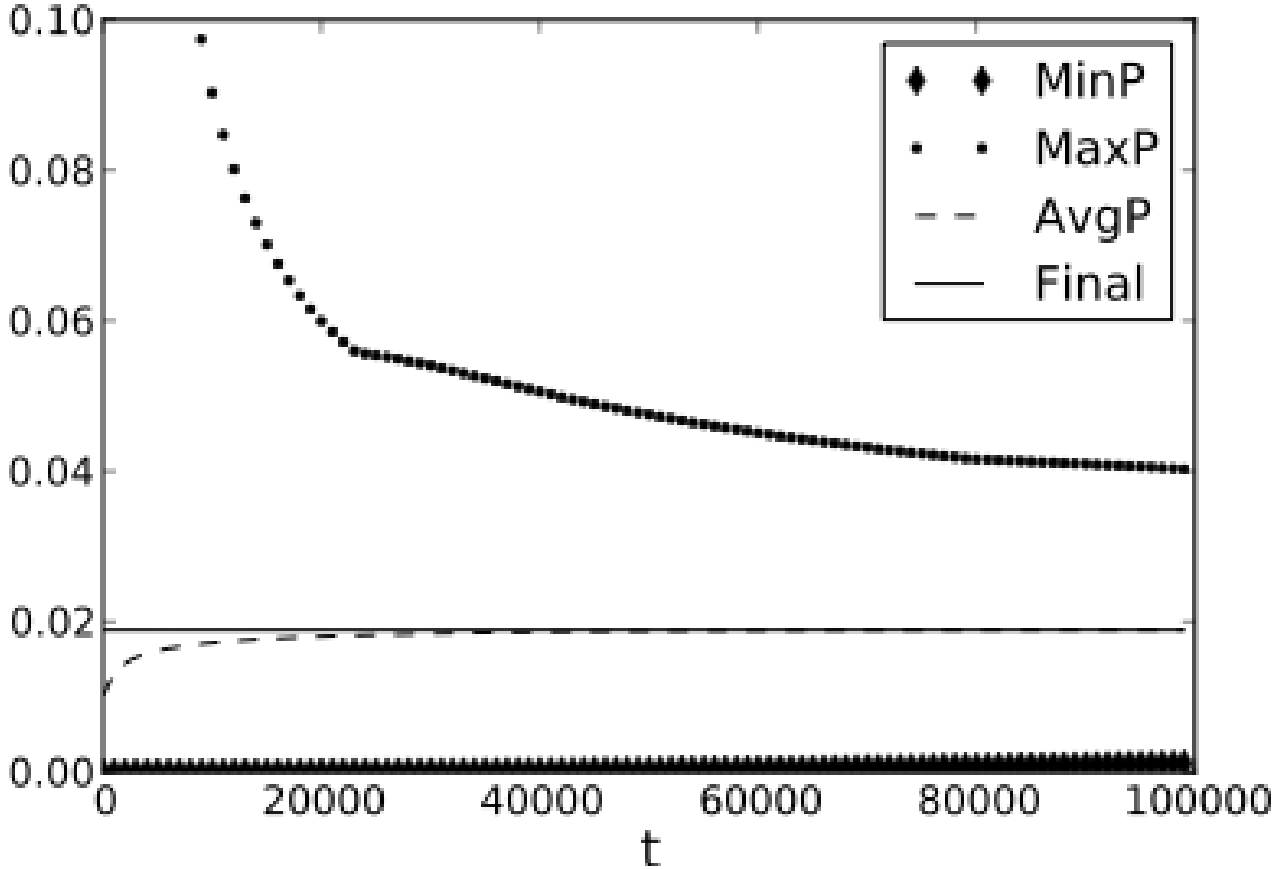
UNIVERSITY OF MARYLAND 1856
Network Science Center
West Point

After 51 Iterations



UNIVERSITY OF MARYLAND 1856
Network Science Center
West Point

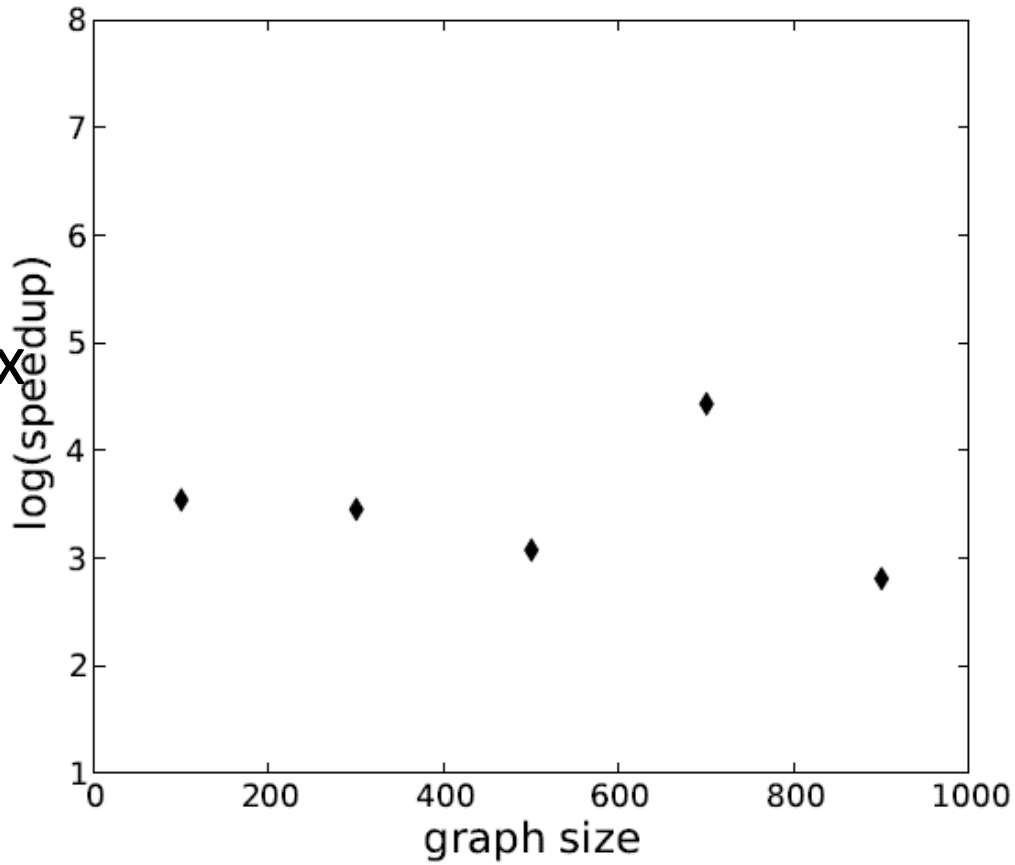
Convergence of Vertex Probabilities



Network Science Center
West Point

Experimental Results

DFP significantly outperforms Monte Carlo simulations by 3x orders of magnitude



University of Maryland 1856

Network Science Center West Point

Conclusions

- Provided a Fast, Deterministic Algorithm To Calculate Fixation Probability on Evolutionary Graphs
  - Works for weighted, directed graphs
  - For r = 1 (neutral drift)
  - Graphs must be Strongly Connected
    - Can we use fix probability of strongly connected sub-graphs to get fixation probability for non-strongly connected graphs?
  - Straight-forward extension to alternative update rules possible

Thank You!

Network Science Center
West Point