# Lecture Notes: Simulation and Markov Chains

In the initial lectures of this course, we sequentially built up a foundational understanding of probability and its applications. The first lecture focused on random number generation and discrete probability, laying the groundwork for our subsequent exploration of random networks. In the third lecture, we navigated the intricacies of Bayes' theorem and conditional probability. Now, as we delve into the current lecture notes, our focus shifts to Markov Chains.

Markov Chains offer a mathematical framework to model systems that evolve from one state to another over time. A typical representation for Markov Chains is a state diagram, as shown in the Figure below.

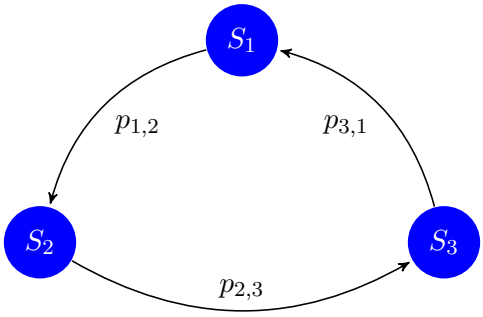



Figure 1: Example of a Markov Chain with three states and transition probabilities.

In the circles represent the states of the system, and the arrows symbolize the potential transitions between these states. The numbers adjacent to the arrows indicate the respective probabilities for these transitions.

As we have traversed through various facets of probability, from the foundational concepts to the applied, it is evident that this journey has prepared us for understanding systems influenced by sequential randomness. In upcoming lectures, we will cap off our discussion by diving into simulations, offering two comprehensive examples: forest fire simulations and ant foraging simulations. These examples will serve as practical applications of the probabilistic and stochastic concepts we have learned so far.

## Markov chains

One of the most fundamental and widely studied stochastic processes is the Markov chain, named after the Russian mathematician Andrey Markov. This chain has a unique property that distinguishes it from other stochastic processes.

**Definition 1** (Markov Chain)**.** *A sequence of random variables* $\{X_0, X_1, X_2, \ldots\}$ *is said to be a Markov chain if, for any* $n \geq 0$ *and any states* $x_0, x_1, \ldots, x_n$*, the probability of the next state* $x_{n+1}$ *depends only on the current state* $x_n$ *and not on the sequence of states preceding it. Mathematically, this property can be expressed as:*

$$P(X_{n+1} = x_{n+1} | X_0 = x_0, X_1 = x_1, \ldots, X_n = x_n) = P(X_{n+1} = x_{n+1} | X_n = x_n)$$

This property is often referred to as the *Markov property* or *memorylessness*. In simpler terms, the future state of a Markov chain depends only on its current state and not on its past states.

**Example 1** (Random Walk)**.** *A random walk is a classic example of a stochastic process and is often used to describe systems or sequences of events where the next state depends only on the*

*current state and some random element. It can be visualized as a path taken by a particle that moves in random directions.*

*The simplest random walk is the one-dimensional walk. At each step, the walker takes a step either to the right (+1) or to the left (-1) with equal probability.*

1. *Start at position 0.*
2. *At each time step, flip a coin:*
   - *If heads, move +1 step to the right.*
   - *If tails, move -1 step to the left.*
3. *Record the position after each step.*
4. *Repeat for a desired number of steps.*


Figure 2: 1D Random Walk over 1000 Steps

*The particle starts at position 0. At each step, it moves either one step to the right (+1) or one step to the left (-1) with equal probability. The path appears quite random, and the particle can drift far from the starting position but can also return close to its starting position at various times.*

*A 2D random walk can be visualized on a grid or plane. At each step, the walker takes a step either up, down, left, or right with equal probability.*

1. *Start at position* $(0, 0)$.
2. *At each time step, randomly choose one of the four directions:*
   - *Up:* $(+0, +1)$
   - *Down:* $(+0, -1)$
   - *Left:* $(-1, +0)$
   - *Right:* $(+1, +0)$
3. *Record the position after each step.*
4. *Repeat for a desired number of steps.*

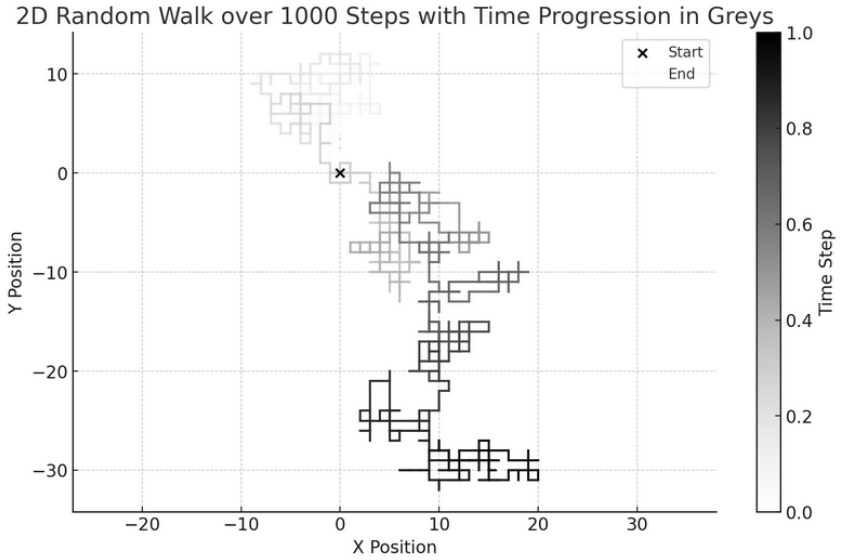



Figure 3: 2D Random Walk over 1000 Steps in Greys

*In the 2D random walk, the particle moves in a plane, starting from the origin. It takes steps in one of four possible directions: up, down, left, or right. The resulting path is a series of connected line segments in the plane, illustrating the random journey of the particle over time. The path is visualized using the 'Greys' color map, where the starting point is black and the ending point is white, representing the time progression.*

**Definition 2.** *For a Markov chain with $N$ possible states, the $N \times N$ matrix $P = [p_{ij}]$ where $p_{ij} = P(X_{n+1} = j | X_n = i)$ is called the transition matrix.*

Note that the rows of a transition matrix for a Markov chain must each sum to 1.

## Characteristics of Markov Chains

1. **Transition Probabilities**: The probabilities of moving from one state to another are called transition probabilities. They are typically represented in a matrix called the transition matrix.

2. **State Space**: The set of all possible states that the chain can be in. This could be a finite or countably infinite set.

3. **Time Structure**: Transitions occur at integer time steps.

**Example 2** (Infection Dynamics)**.** *Consider a population that can be in one of three states: Susceptible (S), Infected (I), and Recovered (R). Individuals transition between these states according to the following Markov chain.*

*The transition probabilities are defined as:*

- $\beta$*: The probability of a Susceptible individual becoming Infected.*
- $\gamma$*: The probability of an Infected individual recovering and moving to the Recovered state.*
- $\sigma$*: The probability of an Infected individual transitioning back to the Susceptible state without recovering.*

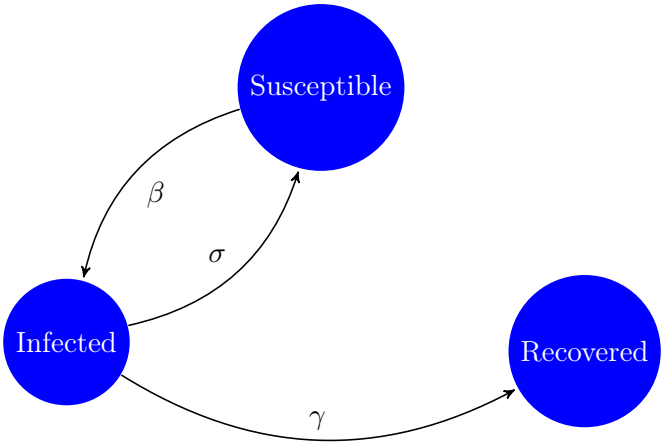



Figure 4: Example of a Markov Chain with three states and transition probabilities.

*Given these probabilities, the transition matrix $P$ for this Markov chain can be constructed as:*

$$P = \begin{bmatrix} 1-\beta & \beta & 0 \\ \sigma & 1-\sigma-\gamma & \gamma \\ 0 & 0 & 1 \end{bmatrix}$$

*Where the rows represent the current state and the columns represent the next state.*

*This Markov chain captures the essential dynamics of many infectious diseases. The future state of each individual depends only on their current state, satisfying the Markov property. For example, if a person is currently Infected, the probability that they will be Recovered in the next time step is $\gamma$, irrespective of their past states.*

Markov chains and graph theory, though distinct in their primary applications, share profound similarities in their mathematical representations. A key point of convergence is the relationship between the transition matrix, central to Markov chains, and the adjacency matrix, foundational in graph theory.

The adjacency matrix, denoted as $A$, is deterministic by nature, with entries either being 0 (indicating no connection) or 1 (indicating a connection between nodes). Its power lies in unveiling potential paths across nodes. Specifically, the entry in row $i$ and column $j$ of $A^n$ (the $n^{th}$ power of $A$) quantifies the number of distinct paths from node $i$ to node $j$ traversing exactly $n$ edges. Thus, for $A$:

$$(A^n)_{ij} = \text{Number of paths from node } i \text{ to node } j \text{ in } n \text{ steps.} \tag{1}$$

Conversely, the transition matrix, $P$, of a Markov chain portrays the likelihood of transitioning between states. Its entries are probabilities, capturing the stochastic nature of the process. To grasp multi-step transitions, one raises $T$ to the $n^{th}$ power:

$$(P^n)_{ij} = \text{Probability of transitioning from state } i \text{ to state } j \text{ in } n \text{ steps.} \tag{2}$$

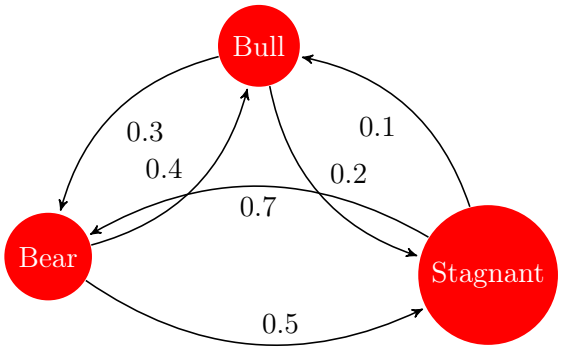
Herein lies a compelling analogy: the adjacency matrix can be seen as a deterministic version of the transition matrix. Its binary values mirror the transition probabilities of either 0 or 1 in $T$. The action of matrix exponentiation further intertwines these concepts with the dimension of time, illuminating paths in networks and evolving probabilities in stochastic processes.

Such parallels accentuate the flexibility of matrix representations: in graph theory, they elucidate network structures; in Markov processes, they depict the dynamic progression of states. This duality offers invaluable insights when maneuvering between deterministic network analyses and probabilistic system dynamics.

**Example 3** (Financial Market Dynamics)**.** *In financial market modeling, a Markov Chain captures the inherent volatility and unpredictability of the market. Here, the future state only depends on the current state, disregarding the historical path.*

***Market States:***

- ***Bull Market (Bull):*** *Optimistic phase with rising or expected-to-rise prices.*
- ***Bear Market (Bear):*** *Pessimistic phase with prolonged price declines.*
- ***Stagnant Market (Stagnant):*** *No clear trend; prices fluctuate within a narrow range.*




***Transition Probabilities:***

- 0.3*: Bull to Bear*
- 0.4*: Bear to Bull*
- 0.2*: Bull to Stagnant*
- 0.1*: Stagnant to Bull*
- 0.5*: Bear to Stagnant*
- 0.7*: Stagnant to Bear*

***Transition Matrix*** $P$***:***

$$P = \begin{pmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.1 & 0.5 \\ 0.1 & 0.7 & 0.2 \end{pmatrix}$$

***Two-Step Transition*** $P^2$***:***

$$P^2 = \begin{pmatrix} 0.39 & 0.32 & 0.29 \\ 0.29 & 0.48 & 0.23 \\ 0.35 & 0.24 & 0.41 \end{pmatrix}$$

***Three-Step Transition*** $P^3$***:***

$$P^3 = \begin{pmatrix} 0.352 & 0.352 & 0.296 \\ 0.360 & 0.296 & 0.344 \\ 0.312 & 0.416 & 0.272 \end{pmatrix}$$

***Interpretation:*** *Transition matrices* $P^2$ *and* $P^3$ *offer insights into the market's longer-term dynamics. For instance, a Bull to Bear transition becomes more probable in three steps, highlighting the dynamic, unpredictable nature of financial markets modeled through Markov Chains.*

## Chapman-Kolmogorov Theorem

Let $P_{ij}^{(n)}$ be the probability that the system transitions from state $i$ to state $j$ in $n$ steps. Then:

$$P_{ij}^{(n)} = P(S_{t+n} = j | S_t = i) = (P^n)_{ij}$$

**Notes:**

- $P_{ij}^{(n)}$ can be found using the $(i, j)$th element of the matrix $P^n$.
- The potential paths from $i$ to $j$ in $n$ steps are up to $m^{n-1}$ ($m$ being the number of states).
- Matrix multiplication of $P$ by itself $n$ times accumulates all transition probabilities.

Another representation of this concept, considering any times $s < t < u$, is given by:

$$P_{ij}(s, u) = \sum_{k \in S} P_{ik}(s, t) \cdot P_{kj}(t, u) \tag{3}$$

**Example 4** (Financial Market Dynamics with Chapman-Kolmogorov Equations)**.** *Consider the previously discussed financial market model. If we're interested in the probability of transitioning from a Bull market to a Bear market over five steps, $P^5$, we can employ the Chapman-Kolmogorov equation. Using our already computed matrices $P^2$ and $P^3$, the equation becomes:*

$$(P^5)_{Bull,\ Bear} = \sum_k (P^2)_{Bull,\ k} \cdot (P^3)_{k,Bear} \tag{4}$$

*Using the above equation, we find that:*

$$(P^5)_{Bull,\ Bear} \approx 0.3526$$

*Here, $k$ represents all possible market states (Bull, Bear, Stagnant). This methodology not only simplifies computations but also offers insights into multi-step transitions in financial markets, enabling better predictive models.*

## Limit Distribution: Irreducibility, Aperiodicity, and Ergodicity

Markov Chains, with their inherent ability to model complex stochastic systems, have significant applications across various domains, from finance and meteorology to social sciences. One of the most pivotal inquiries in the realm of Markov Chains pertains to their long-term behavior. Specifically, will the system stabilize into a steady state or equilibrium? This section delves into the notions that underpin this behavior, including the limit distribution and the properties of irreducibility, aperiodicity, and ergodicity.

**Definition 3** (Limit Distribution)**.** *A distribution $\pi$ is called a limit distribution for a Markov Chain if*

$$\lim_{n \to \infty} P_{ij}(0, n) = \pi_j$$

*for every state $i$. The limit distribution provides insights into the enduring behavior of the system and is inherently linked to the properties discussed below.*

The distribution $\pi$ encapsulates the stable or steady-state probabilities associated with each state as the number of transitions grows indefinitely large. For a finite Markov Chain, the cumulative sum of all elements of $\pi$ equals 1, emphasizing that $\pi$ is a probability distribution.

**Example 5** (Convergence of $P$ to $\pi$)**.** *For the given transition matrix $P$, let's inspect its powers:*

*For $P^5$:*

$$\begin{bmatrix} 0.34296 & 0.35264 & 0.3044 \\ 0.34664 & 0.33984 & 0.31352 \\ 0.33752 & 0.3648 & 0.29768 \end{bmatrix}$$

*For $P^{10}$:*

$$\begin{bmatrix} 0.34260 & 0.35183 & 0.30557 \\ 0.34251 & 0.35210 & 0.30539 \\ 0.34268 & 0.35159 & 0.30573 \end{bmatrix}$$

*For $P^{20}$:*

$$\begin{bmatrix} 0.34259 & 0.35185 & 0.30556 \\ 0.34259 & 0.35185 & 0.30556 \\ 0.34259 & 0.35185 & 0.30556 \end{bmatrix}$$

*By the time we examine $P^{50}$ and $P^{100}$, the matrix has stabilized to:*

$$\begin{bmatrix} 0.34259 & 0.35185 & 0.30556 \\ 0.34259 & 0.35185 & 0.30556 \\ 0.34259 & 0.35185 & 0.30556 \end{bmatrix}$$

*From the matrices above, we discern a clear trend: as we raise $T$ to higher powers, the rows of the matrix are converging to the limit distribution $\pi$. This showcases the theoretical underpinning that, given certain conditions, the Markov Chain will stabilize to a unique long-term distribution.*

**Definition 4.** *A Markov Chain is irreducible if it is possible to traverse from any state to any other state within a finite number of steps. Formally, for any states $i, j \in S$, there exists $n \geq 1$ such that $P_{ij}^{(n)} > 0$.*

Irreducibility plays a paramount role in systems like social networks, ensuring the flow of information across the entire network.

**Definition 5.** *A state of a Markov Chain exhibits aperiodicity if it doesn't revisit itself in a fixed pattern. Formally, a state $i$ is aperiodic if the greatest common divisor of the set of steps $n$ at which it returns to itself is one:* $\gcd\{n : P_{ii}^{(n)} > 0\} = 1$.

Aperiodicity is crucial in financial models to avoid deterministic cyclical behaviors, ensuring the model captures the nuances of real-world dynamics.

**Definition 6.** *A Markov Chain is termed ergodic if it embodies both irreducibility and aperiodicity. Ergodicity ensures the existence of a unique limit distribution $\pi$.*

**Example 6** (Board Game Dynamics)**.** *Consider a simplified board game where players move across a linear track of 10 spaces based on dice rolls. The goal is to reach the 10th space, but there's a catch: the 4th and 7th spaces contain portals. Landing on the 4th space sends the player back to the 1st space, while the 7th space propels the player directly to the 10th space.*

*In this scenario, we can model the game as a Markov Chain, where each space on the board is a state. Transition probabilities depend on dice roll outcomes and the portal mechanics. For instance, if a player is on the 3rd space, there's a $\frac{1}{6}$ chance they'll land on the 4th space (and be sent back to the 1st space) in the next move.*

*The game's dynamics are both irreducible and aperiodic. It's irreducible because a player can move from any space to any other space (either directly or indirectly through dice rolls and portals). It's aperiodic because, while a player may revisit certain spaces multiple times due to the portals, there's no fixed pattern or cycle length for revisiting a specific space.*

*As players play this game repeatedly, we might be interested in the long-term probabilities or limit distribution of a player occupying each space. This distribution will reveal insights like the*

*likelihood of players getting caught in the portal trap at the 4th space or the average number of turns to reach the 10th space. Ergodicity assures us that this distribution will stabilize over time, no matter the starting position.*

In the absence of ergodicity, a Markov Chain might produce vastly divergent outcomes over different simulation runs, complicating predictions and risk assessments. Thus, understanding these attributes is not merely academic; they underpin practical applications across various sectors, playing a crucial role in our understanding of complex systems.

## Forest Fire Simulation as a Markov Chain

The dynamics of forest fires play a pivotal role in ecosystem conservation and the safety of communities adjacent to wooded regions. These fires, influenced by various environmental and situational factors, exhibit intricate patterns of spread, making predictions daunting. However, using mathematical models, especially Markov Chains, we can unravel the stochastic behavior underlying forest fires.

In the Forest Fire Simulation Model, the forest is depicted as a two-dimensional grid, where each cell represents a specific section of the forest. These cells can adopt one of four states: Grass ('G'), Tree ('T'), Burning ('B'), or Empty ('E') which indicates a previously burned area. As the grid evolves in discrete time intervals, the system's behavior aligns with a Markov Chain model, where the subsequent state of each cell hinges exclusively on its present state and the states of its immediate neighbors.

Mathematically, if $G$ denotes the grid and $S_C$ represents the state of a specific cell $C$, then:

$$S_C \in \{\text{Grass}, \text{Tree}, \text{Burning}, \text{Empty}\}$$

The transitions between these states adhere to probabilistic rules:

- A Grass cell has a probability $p_{\text{growth}}$ to metamorphose into a Tree.
- A Tree cell ignites, becoming a Burning cell, if neighboring cells are ablaze, governed by a probability $p_{\text{ignite}}$.
- Occasionally, a Grass cell might spontaneously combust due to rare events like lightning, a phenomenon represented by $p_{\text{spontaneous}}$.
- Post-combustion, a Burning cell invariably transforms into an Empty cell, symbolizing the aftermath of the fire.

These rules can be encapsulated within a transition function $T$, which outlines the state of a cell at time $t+1$ contingent upon its and its neighbors' states at time $t$. This adherence to the Markov property underscores the essence of our model, wherein transitions are strictly influenced by the present state of affairs.

**Experiment 1.** *Our simulation experiment aims to emulate the progression and eventual aftermath of a wildfire in a forest. The grid is initialized with a certain distribution of Grass and Trees, with a few cells set to the Burning state to simulate the fire's ignition points. As the simulation progresses, the fire spreads according to the aforementioned probabilistic rules, affecting neighboring cells and altering the landscape. Over time, the fire exhausts available fuel (Grass and Trees) and transforms cells into the Empty state, representing burned regions. The simulation provides valuable insights into how fires spread, the efficacy of natural barriers, and potential strategies to contain or mitigate wildfires.*

A salient advantage of construing this simulation within the Markov Chain paradigm is the capability to prognosticate the forest's evolution over time. By discerning the steady-state probabilities, we can extrapolate vital data, such as the perennial likelihood of a particular cell being in any given state. Such probabilistic insights are instrumental for forest management strategies, from determining reforestation zones to instituting firebreaks and marshaling firefighting assets.

Additionally, the adaptability of the model shines through its parameters. Probabilities like $p_{\text{growth}}$ and $p_{\text{ignite}}$ can be calibrated to mirror real-world observations or tweaked to simulate myriad scenarios, enhancing the model's versatility.

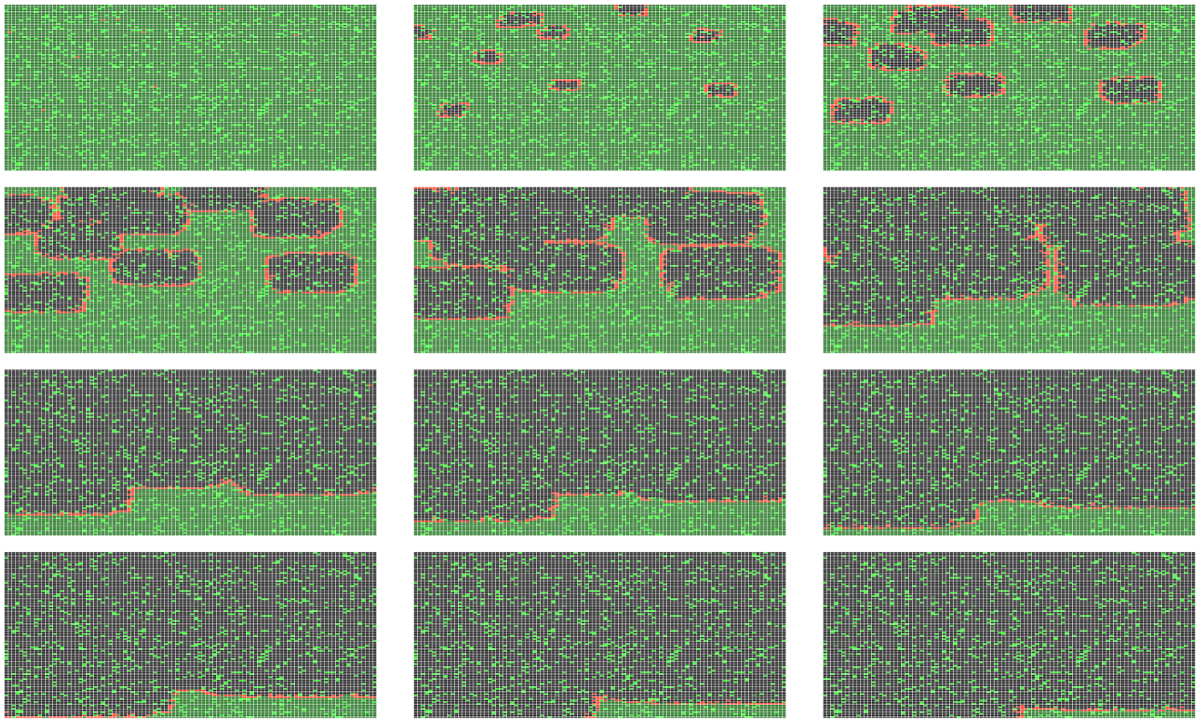


Figure 5: 12 snapshots in the forest fire simulation, showing the dynamic spread and aftermath of the fire.

In summation, Markov Chains furnish a potent methodology for simulating and deciphering the multifaceted dynamics of forest fires. Harnessing their mathematical prowess, we can derive insights into the trajectories of wildfires, optimize resource deployment, and conceive strategies to curtail the ravages of these natural calamities.

## Application: Agent-Based Models

Agent-Based Modeling (ABM) is a computational method used to model and analyze systems composed of individual agents interacting with each other and possibly with their environment. Each agent is typically defined by a set of characteristics and rules governing its behavior. Over time, these individual interactions can lead to the emergence of complex system-wide patterns and behaviors.

In an ABM, agents are often represented as entities with:

- **States**: Described by variables that can change over time, e.g., position, velocity, health status.
- **Behaviors**: Rules or strategies that determine how an agent will act based on its current state and the state of its surroundings.

The environment in which agents operate can be represented as a grid or a network, with agents moving between and interacting within these discrete spaces.

The dynamics of an ABM can often be described by a set of equations. Let $S_i(t)$ represent the state of agent $i$ at time $t$. The behavior of agent $i$ can then be represented as:

$$S_i(t+1) = f(S_i(t), N_i(t))$$

where:

- $f$ is a function describing the agent's behavior.
- $N_i(t)$ represents the neighborhood or set of agents that agent $i$ interacts with at time $t$.

The agents' behaviors and interactions lead to emergent properties of the system, which can be analyzed at the macro level.

The power of ABM lies in its ability to simulate individual behaviors to observe emergent macro-level outcomes. Traditional modeling techniques, such as differential equations, often describe systems at an aggregate level, making it difficult to capture localized interactions and heterogeneity. ABM, on the other hand, provides a bottom-up approach, making it particularly suited for systems where individual behaviors play a critical role in shaping collective dynamics.

**Example 7.** ***Ant Foraging Simulation***

*Consider a grid where ants search for food. The grid has cells representing either food, the nest, pheromones left by other ants, or empty cells. Each ant is an agent with the following behaviors:*

*We provide a computational model to simulate the foraging behavior of ants. The ants' movements are influenced by their environment, primarily the presence of food and pheromones. This document formalizes the rules governing these behaviors based on the provided R code.*

*Let $G$ be the grid where each cell $(i, j)$ represents a position in the 2D space, and $A$ be the set of ants. Each ant $a \in A$ has a state $S_a$ defined as follows:*

$$S_a = \{X, Y, F\}$$

*Where:*

- *$X, Y$ are the coordinates of the ant on the grid.*
- *$F$ is a boolean flag indicating whether the ant is carrying food ($F = 1$) or not ($F = 0$).*

*The state of an ant at time $t + 1$ is given by:*

$$S_{a,t+1} = P(S_{a,t})$$

*Where $P$ is the transition function defined as:*

$$T(S_a) = \begin{cases} (X + \Delta x, Y + \Delta y, 1) & \text{if ant is at food source and } F = 0 \\ (X + \Delta x, Y + \Delta y, 0) & \text{if ant is at nest and } F = 1 \\ (X + \Delta x, Y + \Delta y, F) & \text{otherwise} \end{cases}$$

*$\Delta x$ and $\Delta y$ are random variables that represent the ant's movement in each time step.*

*Ants move based on their current state, previous state, and the state of the cells around them. The movement can be represented as:*

$$M(a_t, a_{t-1}, N(a_t)) \to a_{t+1}$$

*where $a_t$ is the ant's current state at time $t$, $a_{t-1}$ is the previous state, $N(a_t)$ denotes the neighboring cells' states, and $a_{t+1}$ is the resulting state in the next time step.*

*The primary factor affecting the ants' movement is the presence of pheromones. Let's denote pheromones as $Ph_1$ and $Ph_2$. The transition probabilities associated with these pheromones are:*

$$\begin{aligned} P(grass \rightarrow Ph_1) &= p_{grasstopher1} \\ P(Ph_1 \rightarrow Ph_2) &= p_{pher1topher2} \\ P(Ph_2 \rightarrow grass) &= p_{pher2tograss} \\ P(grass \rightarrow P_2) &= p_{grasstopher2} \end{aligned}$$

*When an ant, not carrying food, moves to a cell with food, it picks up the food. This can be represented as:*

$$F(a_t, food) \rightarrow (a_{t+1}, carry)$$

*where $F$ is the function governing food pickup, $a_t$ is the ant's current state, and 'carry' indicates the ant is now carrying food.*

*Ants carrying food, when they move and are not at the nest or on a food source, drop a pheromone. This can be represented as:*

$$P(a_t, carry) \rightarrow P_1$$

*Over time, pheromones on the grid undergo transitions:*

$$\begin{aligned} Ph_1 \rightarrow Ph_2 \quad & with\ probability\ p_{pher1topher2} \\ Ph_2 \rightarrow grass \quad & with\ probability\ p_{pher2tograss} \end{aligned}$$

*The randomness in ant movement is influenced by transition probabilities. Given a certain probability $p$, an ant will transition from state $x$ to state $y$. This is represented by:*

$$P(x, y, p) = \begin{cases} y & with\ probability\ p \\ x & otherwise \end{cases}$$

*The simulation environment, including the ant positions, food sources, and nest, is initialized. The grid contains various entities: grass, ants, nest, and food.*