*EN-625.664.81.SP21 COMPUTATIONAL STATISTICS*

COURSE PROJECT

# SIR Epidemiology Model in a Homogeneous Population by Adaptive Markov Chain Monte Carlo (MCMC)

**By Ricca Callis**

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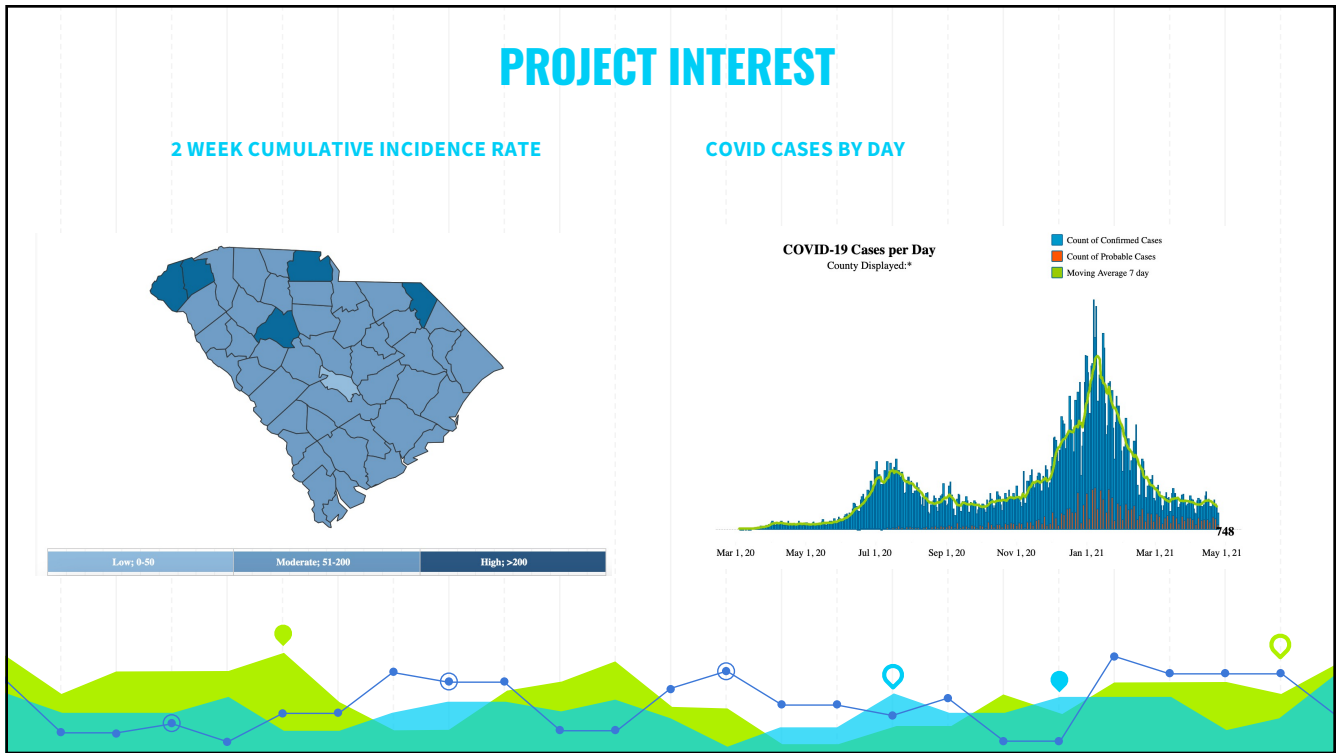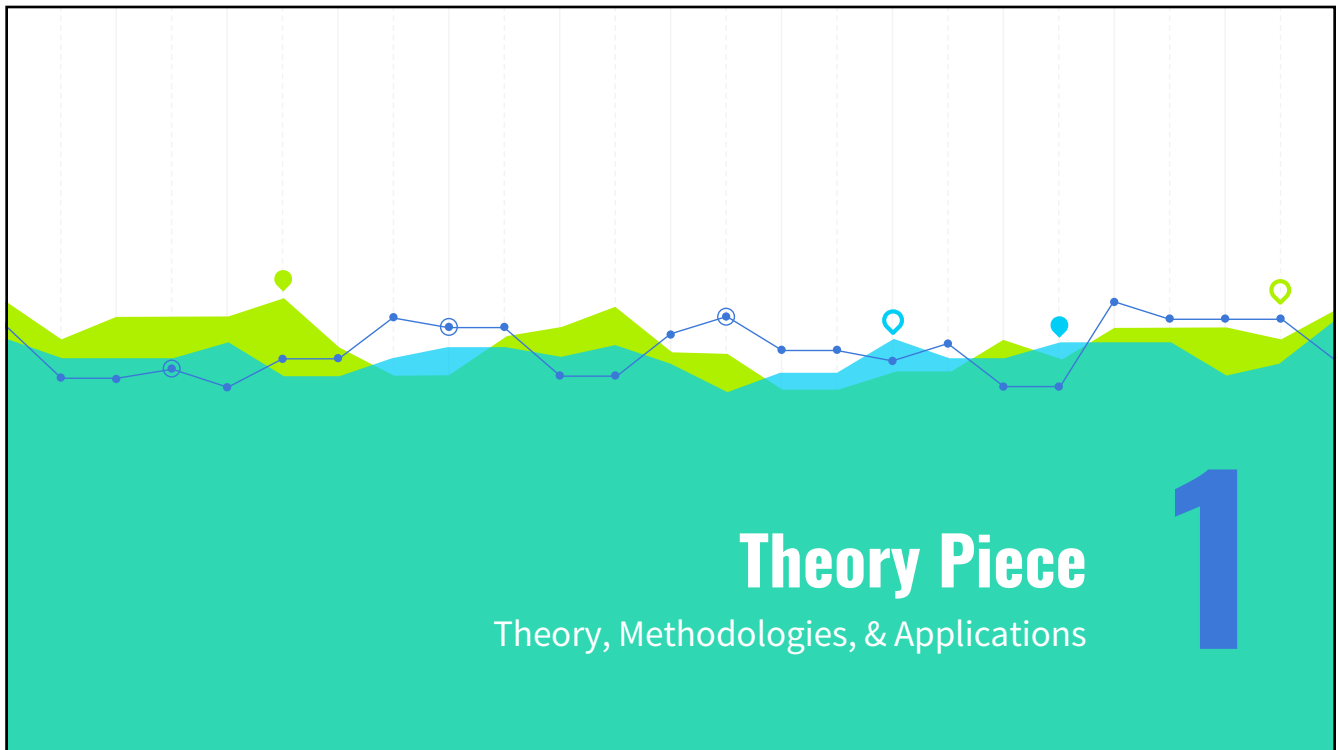# HELLO!

## I am Ricca Callis

Managing BMH COVID-19 Vaccine Clinic & Mobile Testing Unit
has inspired this course project

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# PROJECT INTEREST

**2 WEEK CUMULATIVE INCIDENCE RATE**

**COVID CASES BY DAY**

**COVID-19 Cases per Day**
County Displayed:*

Count of Confirmed Cases
Count of Probable Cases
Moving Average 7 day

748

Mar 1, 20    May 1, 20    Jul 1, 20    Sep 1, 20    Nov 1, 20    Jan 1, 21    Mar 1, 21    May 1, 21

Low; 0-50    Moderate; 51-200    High; >200

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# Theory Piece
Theory, Methodologies, & Applications

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# COMPARTMENTAL MODEL FRAMEWORK

- ◉ Model: Differential equations of dynamic systems
- ◉ Compartment:
    - ○ Abstract entity representing the quality of interest
    - ○ Equivalent to a system state
    - ○ Visually conceptualized as a box
    - ○ Internally homogeneous
- ◉ Compartment Interactions: Through a set of rate equations
    - ○ Visually conceptualized by arrows between compartments
- ◉ Net Flow Into a Compartment: A set of first order linear or nonlinear equations

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# COMPARTMENTAL MODEL FRAMEWORK

For an n compartment system,

- ◉ Compartment/state variables    $x(t) = [x_1(t), \dots, x_n(t)]^T$
- ◉ State-space model:

$$\dot{x}(t) = f(x(t), w(t); \theta(t), t)$$
$$y(t) = g(x(t); \theta(t), t) + v(t)$$

- ◉ where,

$f(\cdot)$ is the state dynamics function corresponding to the compartmental model

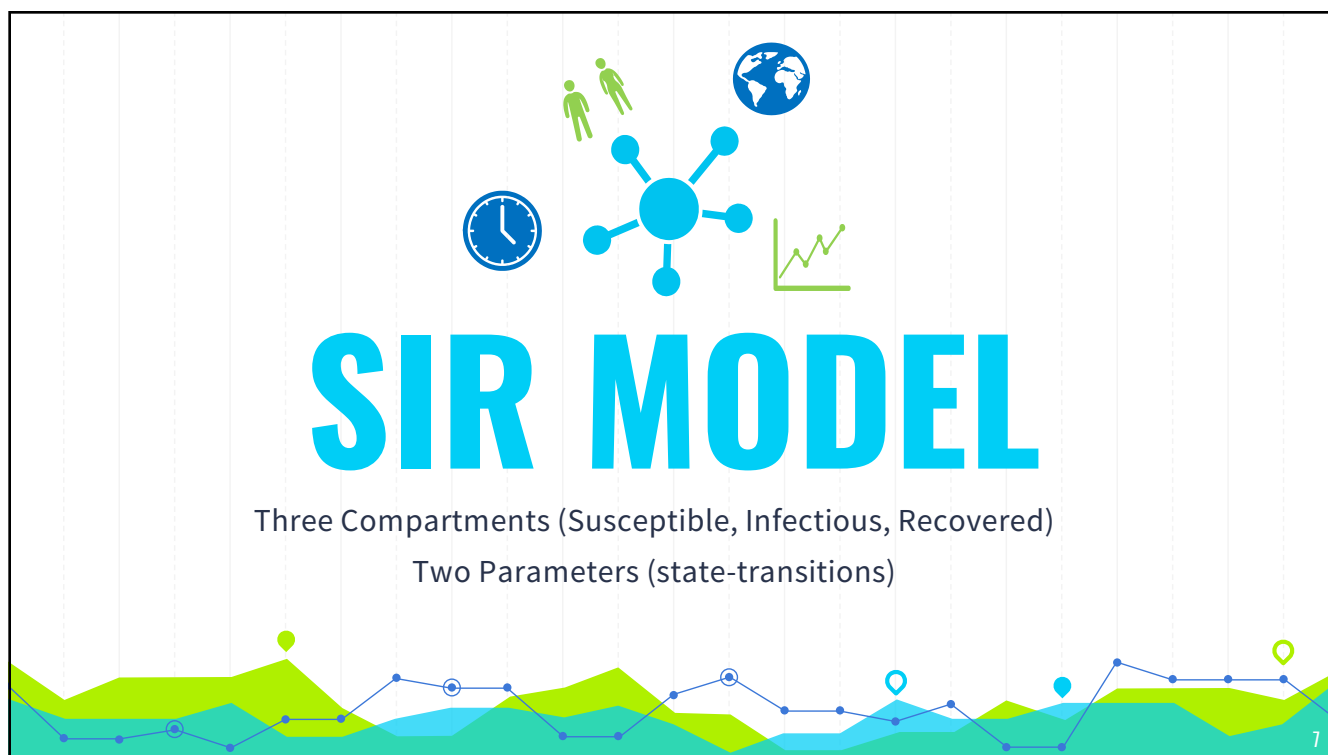$w(t) = [w_1(t), \dots, w_1(t)]^T$ is the external system inputs

$y(t) = [y_1(t), \dots, y_m(t)]^T$ is the vector of observable model invariables (i.e., outputs)

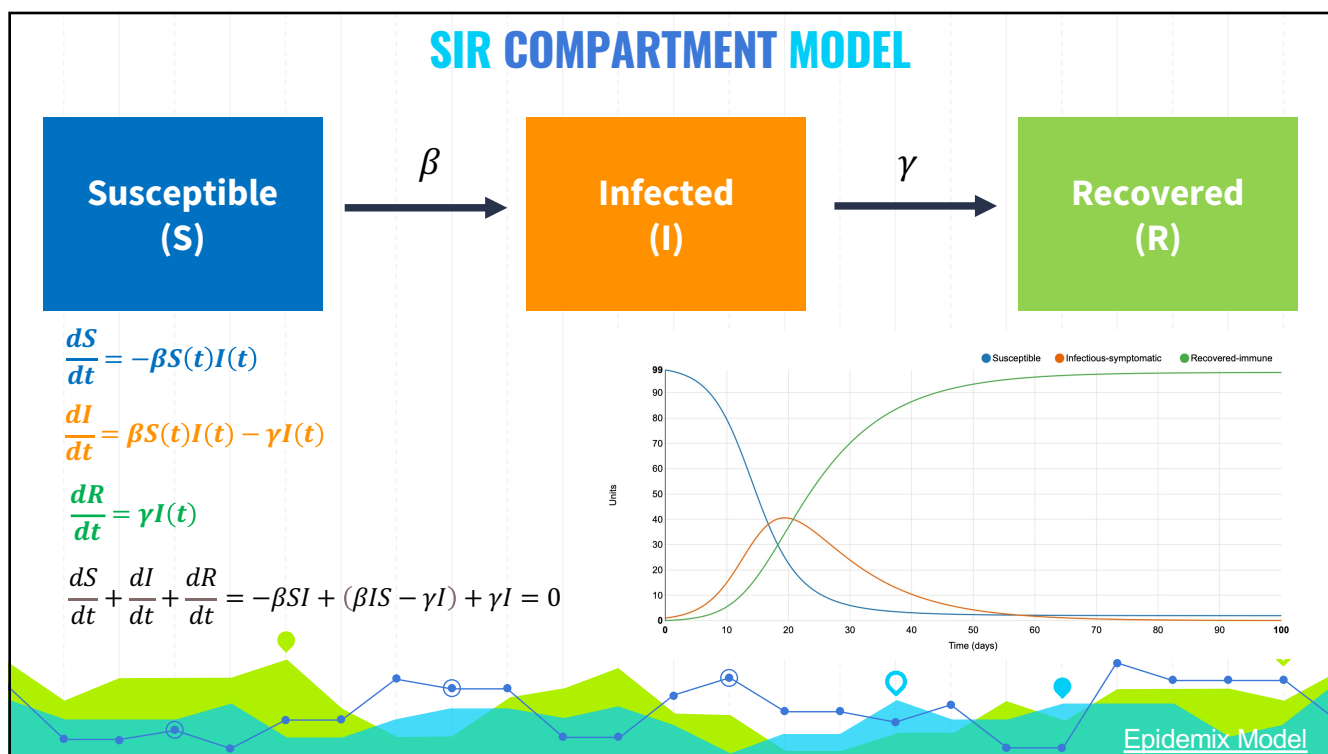$g(\cdot)$ is the function that maps state variables to observations (measurements)

$v(t) = [v_1(t), \dots, v_m(t)]^T$ is the vector of measurement error

$\theta(t) = [\theta_1(t), \dots, \theta_p(t)]^T$ is the vector of model parameters to be set or identified

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# SIR MODEL

Three Compartments (Susceptible, Infectious, Recovered)

Two Parameters (state-transitions)

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# SIR COMPARTMENT MODEL

| Susceptible (S) | $\xrightarrow{\beta}$ | Infected (I) | $\xrightarrow{\gamma}$ | Recovered (R) |

$$\frac{dS}{dt} = -\beta S(t)I(t)$$

$$\frac{dI}{dt} = \beta S(t)I(t) - \gamma I(t)$$

$$\frac{dR}{dt} = \gamma I(t)$$

$$\frac{dS}{dt} + \frac{dI}{dt} + \frac{dR}{dt} = -\beta SI + (\beta IS - \gamma I) + \gamma I = 0$$

Epidemix Model

# SIR MODEL PARAMETERS

- ◉ $\beta$: Transmission parameter
  - ○ Depends on effective contact per unit of time
  - ○ Most important parameter, but difficult to estimate directly
  - ○ Can be estimated if we assume individuals mix randomly: $\beta = \frac{R_0}{ND}$ (where D is duration of infectiousness)
- ◉ $R_0$ : Reproductive number
  - ○ A measure of how infectious the disease is
  - ○ The average number of new infected individuals caused by one infectious individual.
  - ○ Can be estimated by fitting model predictions to observed data: $R_0 = \frac{\beta S_0}{\gamma}$ (where $S_0$ is the initial number of susceptible individuals)
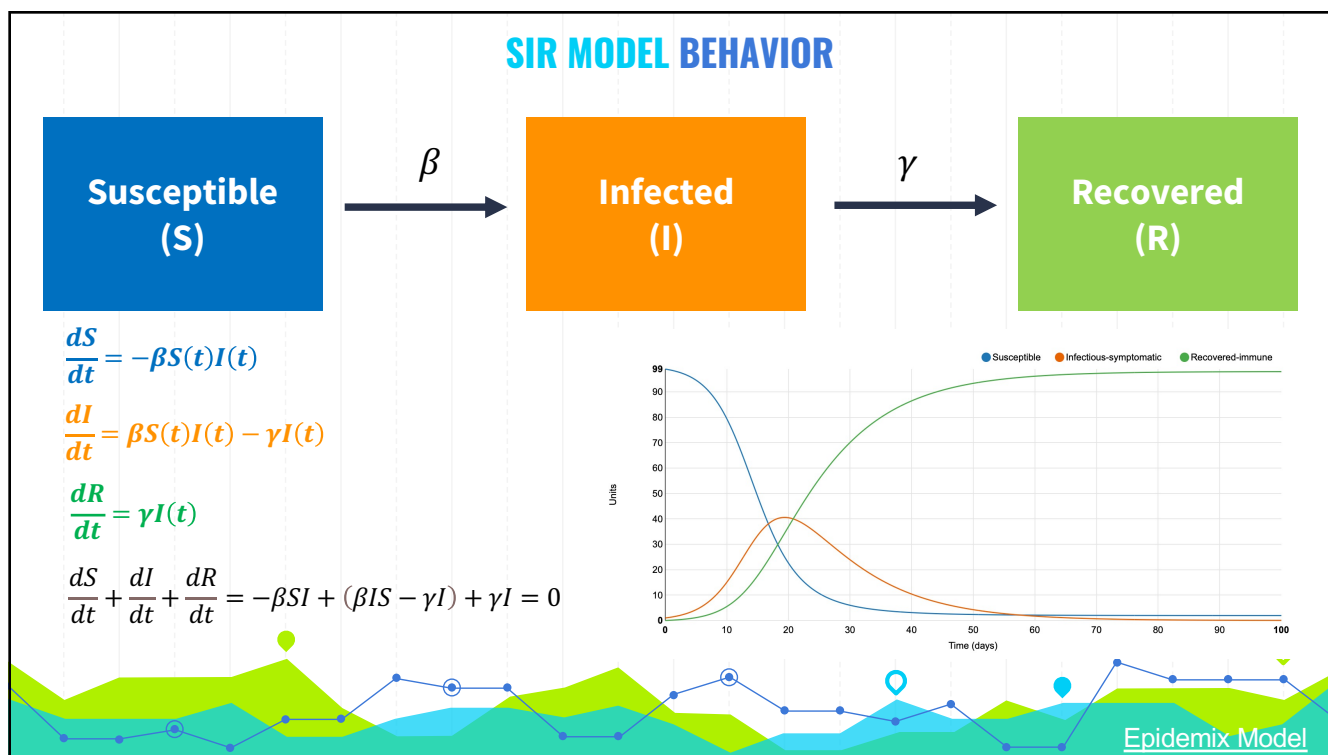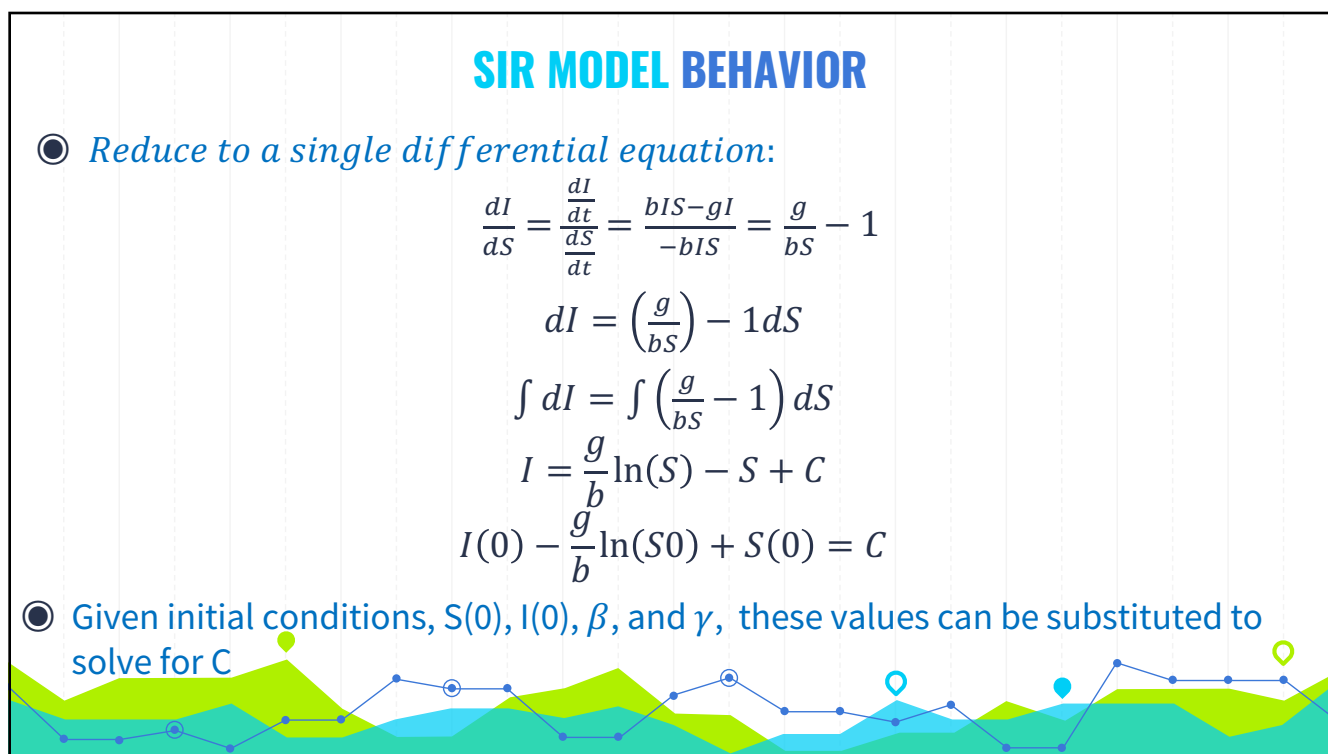
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# SIR MODEL BEHAVIOR

- ◉ $R_0$ : Reproductive number
  - ○ clearly affected by both transmission ($\beta$) and recovery ($\gamma$) rates.
  - ○ When $R_0$ >1, the occurrence of the disease will increase.
    - • Here, I($t$) increases, reaches a maximum, and then decreases to zero as $t \rightarrow \infty$.
  - ○ When $R_0$ < 1, the occurrence of the disease will decrease and eventually die out.
    - • Here, I($t$) decreases monotonically to zero as $t \rightarrow \infty$.
  - ○ However, when $R_0$ = 1, the disease occurrence will remain constant.
  - ○ We can see that values of $R_0$ close to 1 produce very slow-growing epidemics, while values of $R_0$ much greater than one produce fast, explosive epidemics.

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# SIR MODEL BEHAVIOR



$$\frac{dS}{dt} = -\beta S(t)I(t)$$

$$\frac{dI}{dt} = \beta S(t)I(t) - \gamma I(t)$$

$$\frac{dR}{dt} = \gamma I(t)$$

$$\frac{dS}{dt} + \frac{dI}{dt} + \frac{dR}{dt} = -\beta SI + (\beta IS - \gamma I) + \gamma I = 0$$

Epidemix Model

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# SIR MODEL BEHAVIOR

◉ *Reduce to a single differential equation:*

$$\frac{dI}{dS} = \frac{\frac{dI}{dt}}{\frac{dS}{dt}} = \frac{bIS - gI}{-bIS} = \frac{g}{bS} - 1$$

$$dI = \left(\frac{g}{bS}\right) - 1 \, dS$$

$$\int dI = \int \left(\frac{g}{bS} - 1\right) dS$$

$$I = \frac{g}{b}\ln(S) - S + C$$

$$I(0) - \frac{g}{b}\ln(S0) + S(0) = C$$

◉ Given initial conditions, S(0), I(0), $\beta$, and $\gamma$, these values can be substituted to solve for C

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# SIR MODEL BEHAVIOR

◉ How the compartmentalized groups will act as $t \to \infty$
- ○ Susceptible group will decrease over time and approach 0
- ○ Recovered group will increase and approach population size (N)
- ○ The rate of change for the infected group depends on $\beta, \gamma$, and S(t).
  - ○ When $\beta S(t)$ is less than $\gamma$: the rate of change for the infected group is negative.
  - ○ When $\beta S(t)$ is greater than $\gamma$: the rate of change for the infected group is positive.
  - ○ When $\beta S(t)$ is equal to $\gamma$: the rate of change for the infected/infectious group is zero.
- ○ The disease always dies out
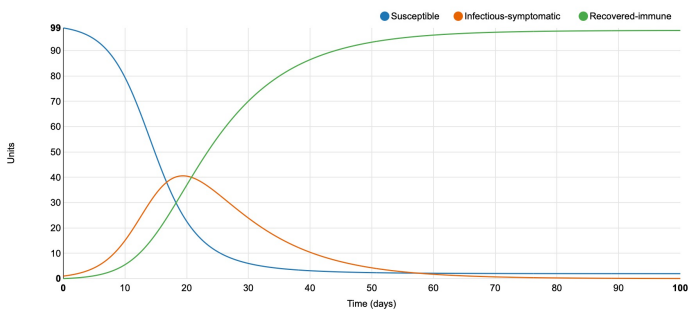
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# LINKING MODEL TO DATA



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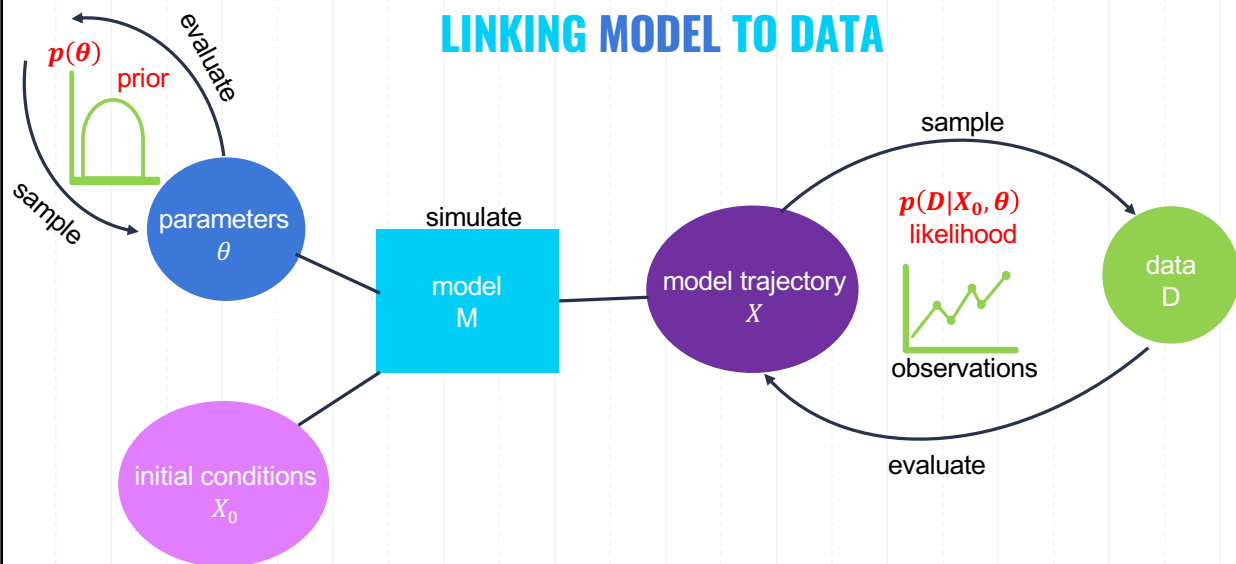
# BAYESIAN INFERENCE

- ◉ Calculate the posterior $p(\theta|data)$
    - ○ Inherent uncertainty in parameters
    - ○ Posterior is the probability distribution of a random variable $\theta$
- ◉ Bayes' Rule $p(\theta|data) = \frac{p(data|\theta)p(\theta)}{p(data)}$
    - ○ $p(\theta|data)$ is the posterior
    - ○ $p(data|\theta)$ is the likelihood
    - ○ $p(\theta)$ is the prior
    - ○ $p(data)$ is the normalization constant
- ◉ i.e., $(posterior) \propto (normalization\ likelihood) \cdot (prior)$

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# BAYESIAN INFERENCE

- ◉ Expectation Values
    - ○ Parameter(s) $\theta$ are interpreted as a random variable, distributed according to the posterior: $p(\theta|data) \propto p(data|\theta)p(\theta)$
    - ○ We want to generate samples of $\theta$ from this distribution
    - ○ To calculate the expected value of any quantity, given the data, we integrate over $p(\theta)$: $E[A] = \int p(\theta|data)X(\theta)d\theta$
    - ○ E.g., for SIR model, if we know $p(\beta, \gamma)$, we can calculate the expected value of $R_0$: $E[R_0] = \int p(\beta, \gamma|data)\frac{\beta}{\gamma}d\beta d\gamma$

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## BAYESIAN INFERENCE

◉ Sample Approximation

- ○ How do we find an expression for $p(\beta, \gamma | data)$?
- ○ Monte-Carlo approximation:

$$\int f(x)p(x)dx \approx \sum_x p(x)f(x)$$

- ○ Or, draw N samples from $p(x)$ and calculate

$$\int f(x)p(x)dx \approx \frac{1}{N} \sum_{x \sim p(x)} f(x)$$

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# MARKOV CHAIN MONTE CARLO

A chain of samples where each proposed $\theta^*$ depends on the previous one

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# MARKOV CHAIN MONTE CARLO (MCMC)

◉ Markov chain: stochastic sequence of states in which the next state depends only upon the current state $\theta_{t+1} \sim \mathbb{D}(\theta_t)$

◉ Algorithms generates a sequence of parameter values $\theta_1, \theta_2, \dots$ , whose empirical distribution, approaches the posterior distribution.

◉ The generation of the vectors in the chain, is done by random numbers (Monte Carlo) in such way that each new point may only depend on the previous point (Markov chain).

　　○ The chain is used as if it is a sample from the posterior.

◉ Metropolis-Hastings Algorithm: a particular way of using MCMC to sample from a distribution

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# METROPOLIS-HASTINGS ALGORITHM

◉ Generate a Markov chain with a transition density

$$p(\theta, \theta^*) = q(\theta, \theta^*)\alpha(\theta, \theta^*), \theta \neq \theta^*$$

$$p(\theta, \theta) = 1 - \int q(\theta, \theta^*)\alpha(\theta, \theta^*)d\theta$$

For some proposal density q and for acceptance probability $\alpha$

◉ The chain is reversible IFF

$$f(\theta)q(\theta, \theta^*)\alpha(\theta, \theta^*) = f(\theta^*)q(\theta^*, \theta)\alpha(\theta^*, \theta)$$
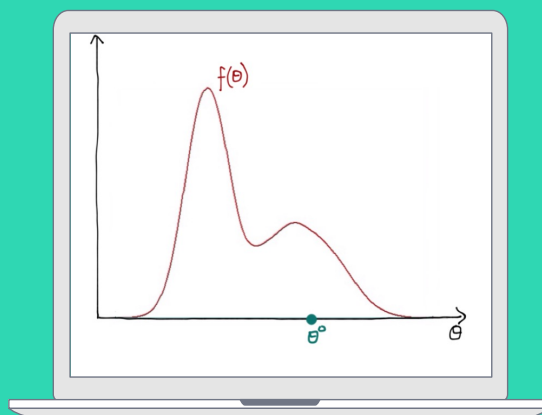
◉ Thus, we choose $\alpha$ as

$$\alpha(\theta, \theta^*) = min\left\{1, \frac{f(\theta^*)q(\theta^*, \theta)}{f(\theta)q(\theta, \theta^*)}\right\}$$
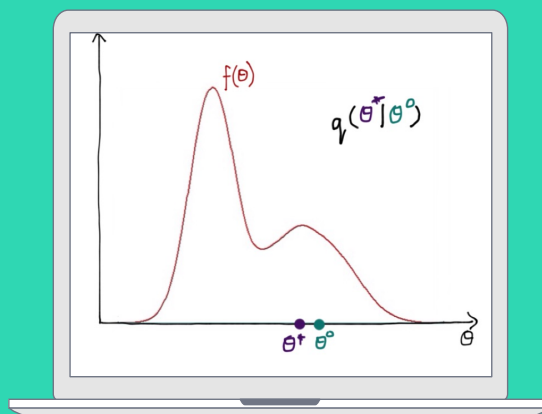
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# METROPOLIS-HASTINGS ALGORITHM

1. Initialize $\theta^0$ and proposal density $q$, set $\theta = \theta^0$



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# METROPOLIS-HASTINGS ALGORITHM

1. Initialize $\theta^0$ and proposal density $q$, set $\theta = \theta^0$
2. Sample $\theta^* \sim q(\theta^*|\theta)$



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8/2/21

# METROPOLIS-HASTINGS ALGORITHM

1. Initialize $\theta^0$ and proposal density $q$, set $\theta = \theta^0$
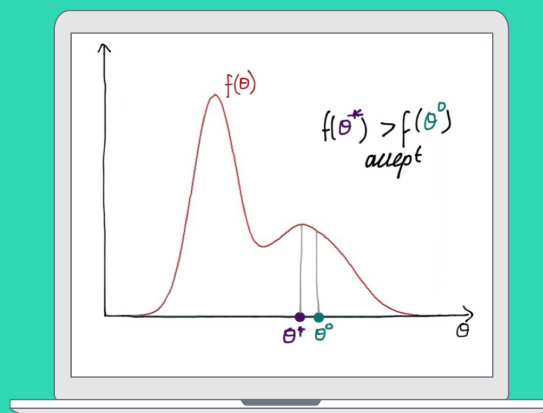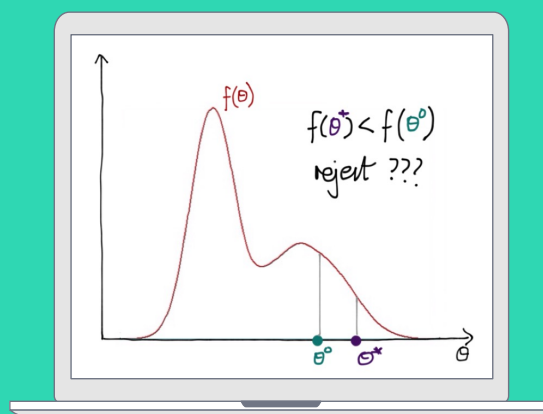
2. Sample $\theta^* \sim q(\theta^*|\theta)$

3. Compute acceptance probability, r

   **ACCEPTANCE**
   - **If $q(\theta^*|\theta)$ symmetric, then**
     $$r = min\left(1, \frac{f(\theta^*)}{f(\theta)}\right)$$
   - **Move to $\theta^*$ if more probable than $\theta$**



$f(\theta)$

$f(\theta^*) > f(\theta^0)$
accept

$\theta^*$ $\theta^0$

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# METROPOLIS-HASTINGS ALGORITHM

1. Initialize $\theta^0$ and proposal density $q$, set $\theta = \theta^0$

2. Sample $\theta^* \sim q(\theta^*|\theta)$
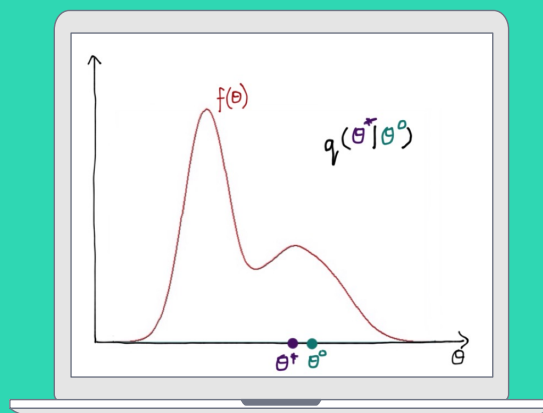
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   - **If $q(\theta^*|\theta)$ symmetric, then**
     $$r = min\left(1, \frac{f(\theta^*)}{f(\theta)}\right)$$
   - **Move to $\theta^*$ if more probable than $\theta$**
   - **If $q(\theta^*|\theta)$ asymmetric, then**
     $$r = min\left(1, \frac{f(\theta^*)q(\theta|\theta^*)}{f(\theta)q(\theta^*|\theta)}\right)$$



$f(\theta)$

$f(\theta^*) < f(\theta^0)$
reject ???

$\theta^0$ $\theta^*$

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# METROPOLIS-HASTINGS ALGORITHM

1. Initialize $\theta^0$ and proposal density $q$, set $\theta = \theta^0$

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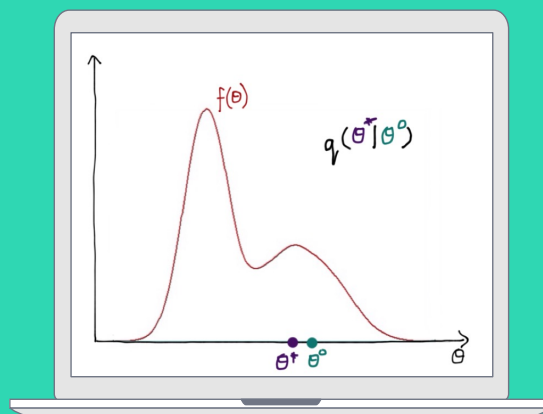   - **If $q(\theta^*|\theta)$ asymmetric, then**
     $$r = min\left(1, \frac{f(\theta^*)q(\theta|\theta^*)}{f(\theta)q(\theta^*|\theta)}\right)$$

4. Draw $u \sim Uniform[0,1]$



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# METROPOLIS-HASTINGS ALGORITHM

1. Initialize $\theta^0$ and proposal density $q$, set $\theta = \theta^0$

2. Sample $\theta^* \sim q(\theta^*|\theta)$

3. Compute acceptance probability, r
   **ACCEPTANCE**
   - **If $q(\theta^*|\theta)$ symmetric, then**
     $$r = min\left(1, \frac{f(\theta^*)}{f(\theta)}\right)$$
   - **Move to $\theta^*$ if more probable than $\theta$**
   - **If $q(\theta^*|\theta)$ asymmetric, then**
     $$r = min\left(1, \frac{f(\theta^*)q(\theta|\theta^*)}{f(\theta)q(\theta^*|\theta)}\right)$$

4. Draw $u \sim Uniform[0,1]$

5. Set new sample to

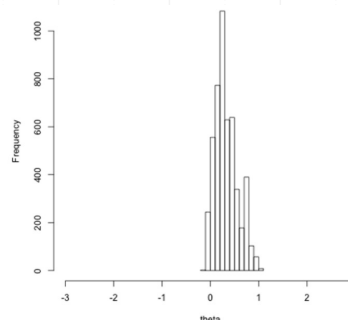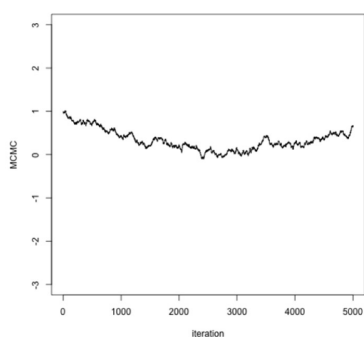$$\theta_{i+1} = \begin{cases} \theta^*, if\ u<r \\ \theta_i, if\ u \geq r \end{cases}$$
6. Repeat sets 2-5
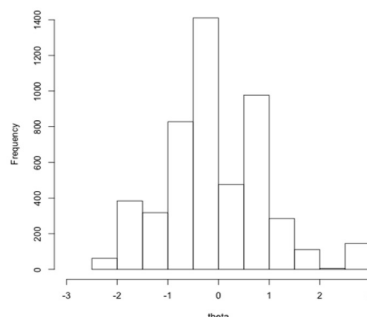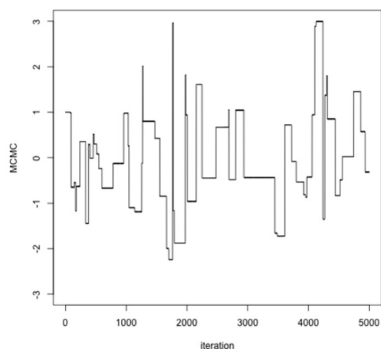


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# CHOOSING A PROPOSAL DISTRIBUTION :"GOLDIE LOCKS"

◉ If variance is too small, the chain will be slow to reach the target distribution



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# CHOOSING A PROPOSAL DISTRIBUTION: "GOLDIE LOCKS"
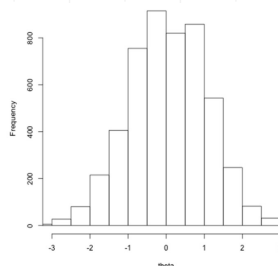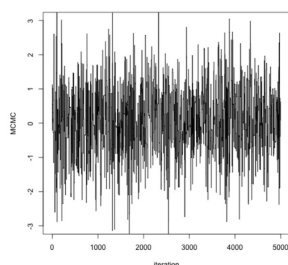
◉ If variance is too high, many proposed values will be rejected and the chain will stick in one place for many steps



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# CHOOSING A PROPOSAL DISTRIBUTION: "GOLDIE LOCKS"

◉ If variance is just right, the chain will efficiently explore the full shape of the target distribution



◉ We can either:
  ○ Trial and Error: Try several different proposal distributions (pilot runs) , aiming for acceptance rate of 24-40%
  ○ Use Adaptive MCMC

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# ADAPTIVE MCMC

◉ New point depends on previous point AND on earlier history of the chain
◉ The adaptation is based on an increasing part of the chain
◉ Uses a Gaussian proposal with covariance $C_n$ that depends on the chain generated so far:

$$C_n = \begin{cases} C_0, & n \le n_0 \\ s_d cov(\theta_1, \dots, \theta_n) + s_d \varepsilon I_d, & n > n_0 \end{cases}$$

◉ Where

  $s_d$ is a parameter that depends only on the dimension $d$ of the sample space (usually $s_d = 2.4^2/d$)

  $\varepsilon > 0$ is a constant we keep very small

  $n_0 > 0$ is the length of the initial nonadaptive period

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## SUMMARY POINTS

◉ SIR Compartmental Model
◉ Likelihood as $p(data|\theta)$ to express closeness of model to data
◉ Bayesian inference: $(posterior) \propto (normalized\ likelihood) \cdot (prior)$
◉ To estimate quantities or project into the future, need to calculate.
$E[A] = \int p(\theta|data)X(\theta)d\theta$
◉ Monte Carlo sampling as a method to calculate this
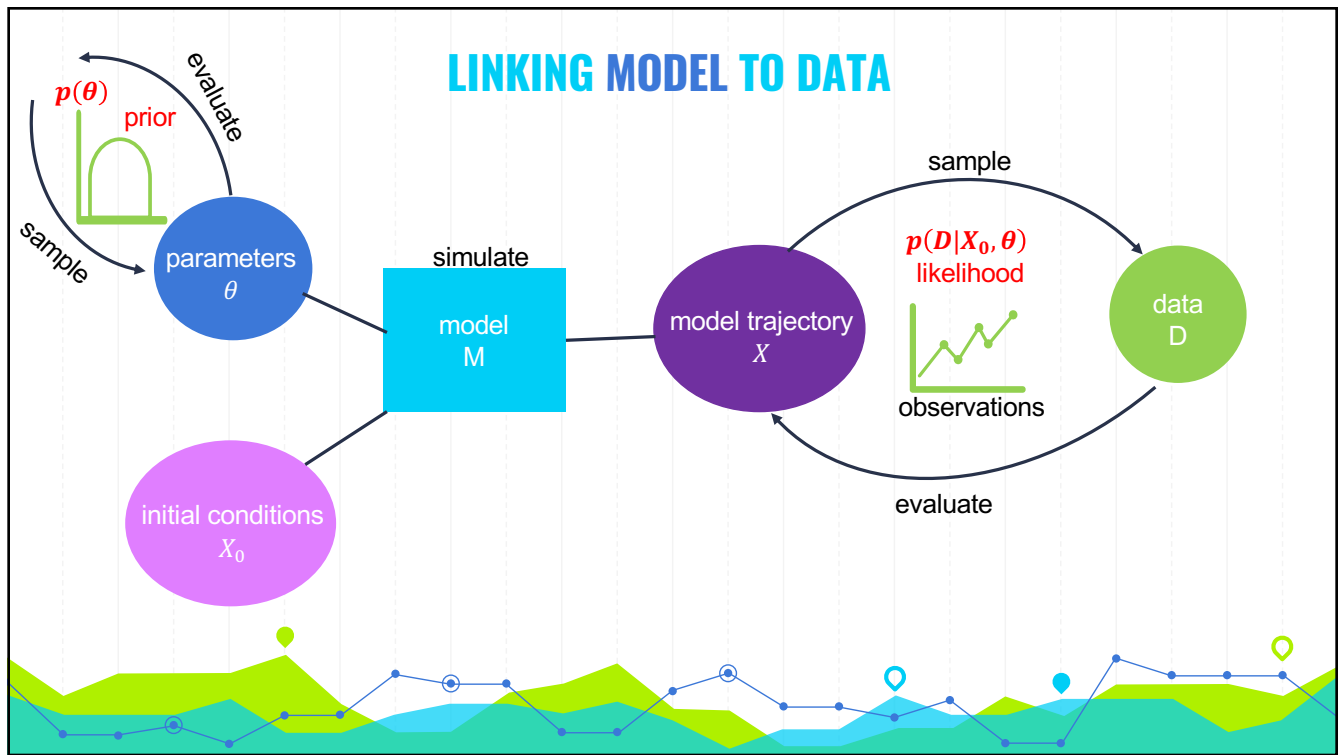◉ Use Metropolis-Hastings Markov-Chain Monte Carlo Method
◉ Adaptive MCMC

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# Computational Piece 2
Programmed Computational Example (Code, Output, & Graphs)

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# LINKING MODEL TO DATA

$p(\theta)$
prior

evaluate

sample

parameters
$\theta$

initial conditions
$X_0$

model
M

simulate

model trajectory
$X$

sample

$p(D|X_0, \theta)$
likelihood

observations

evaluate

data
D

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# COMPUTATIONS (CODE)

◉ R Video

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**The End!** 3

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# THANKS FOR WATCHING!

## Any questions?
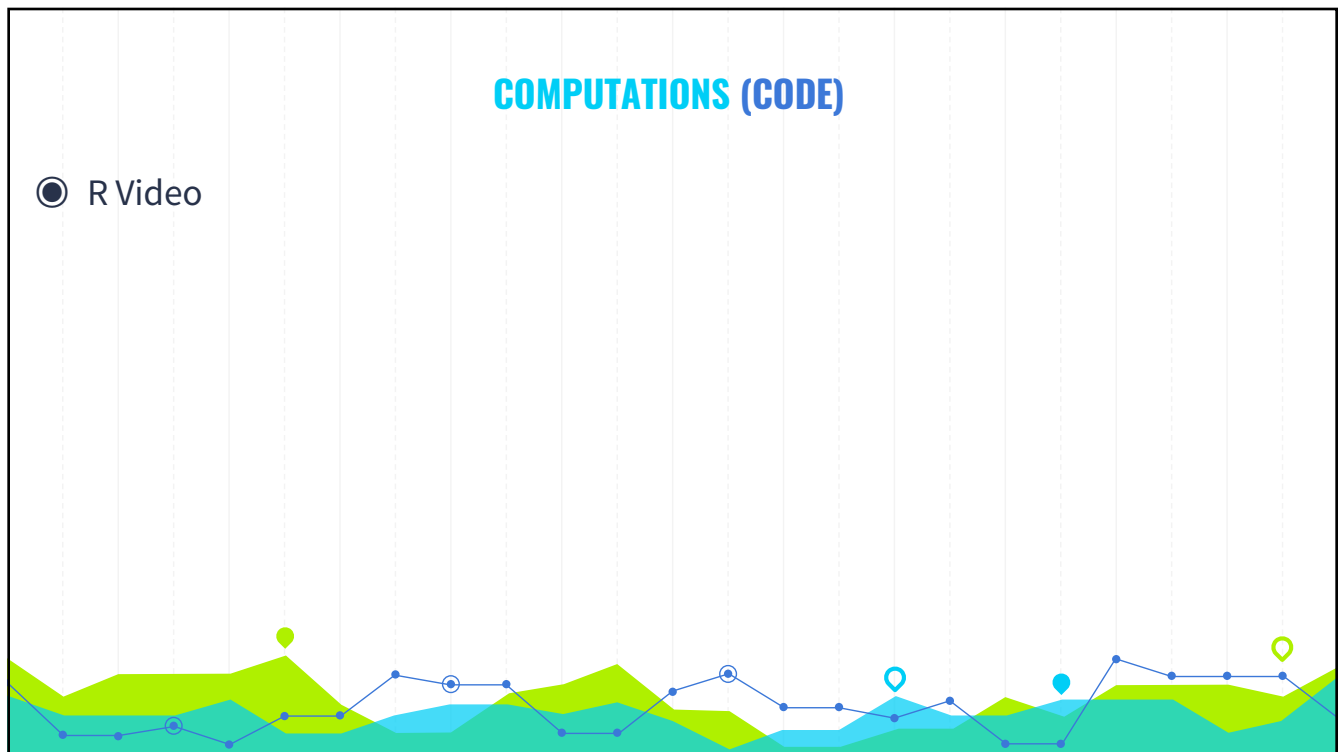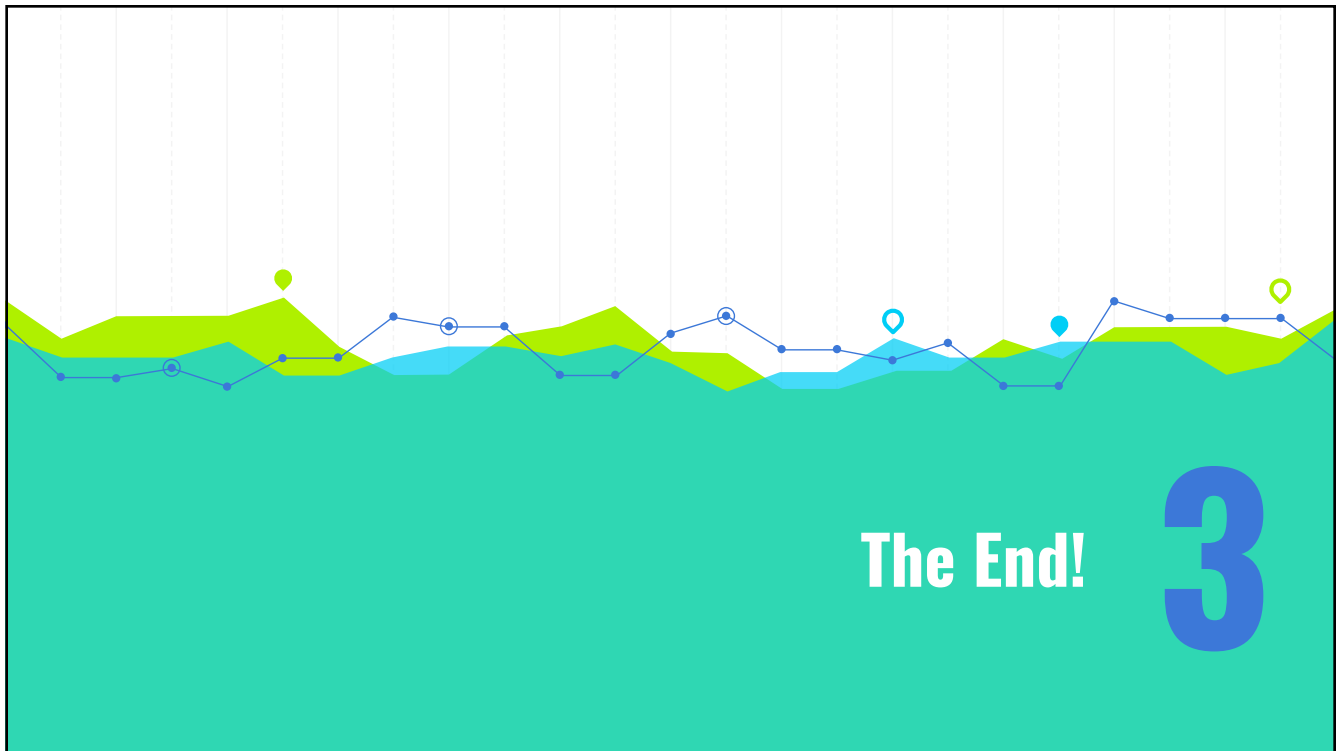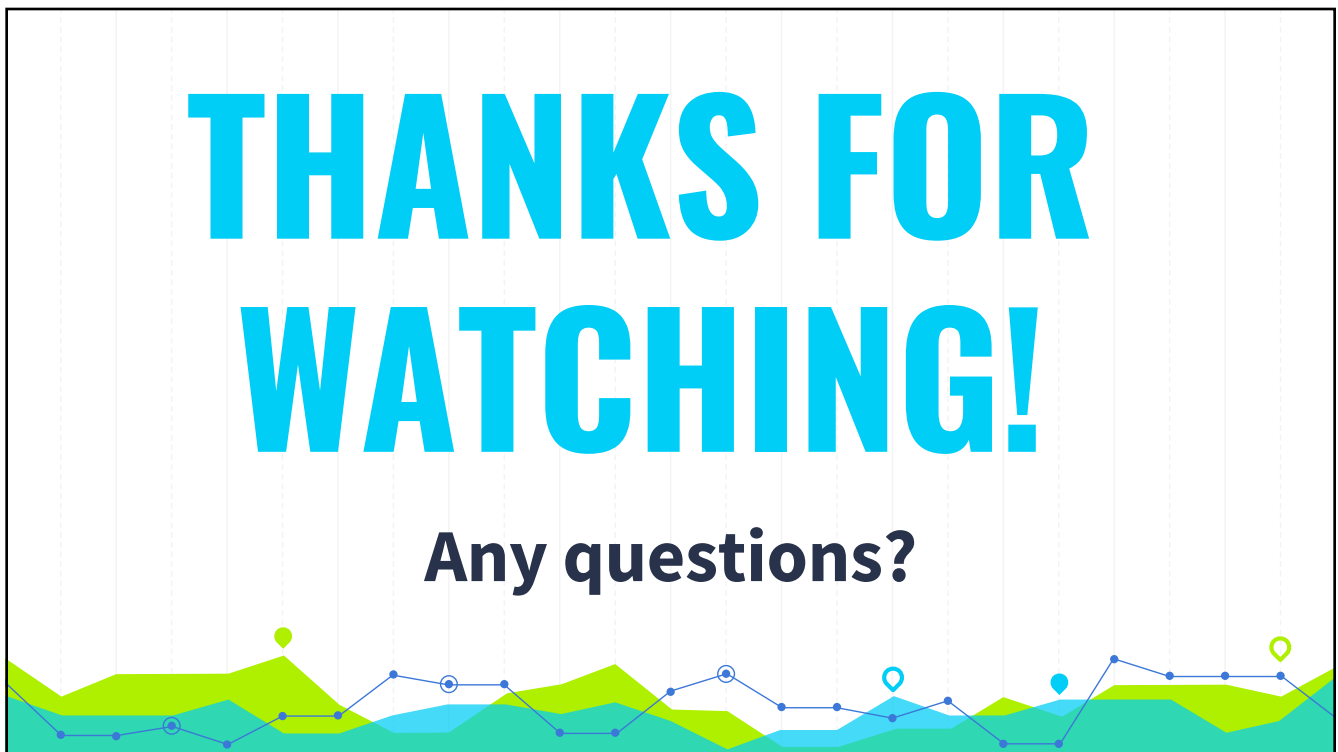
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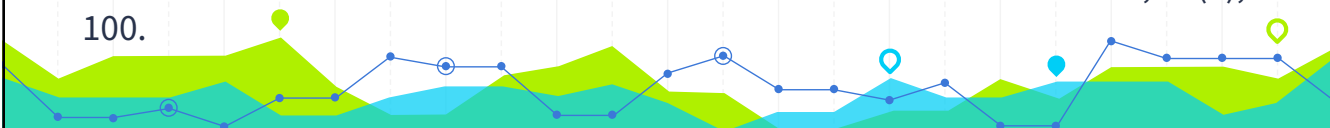
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