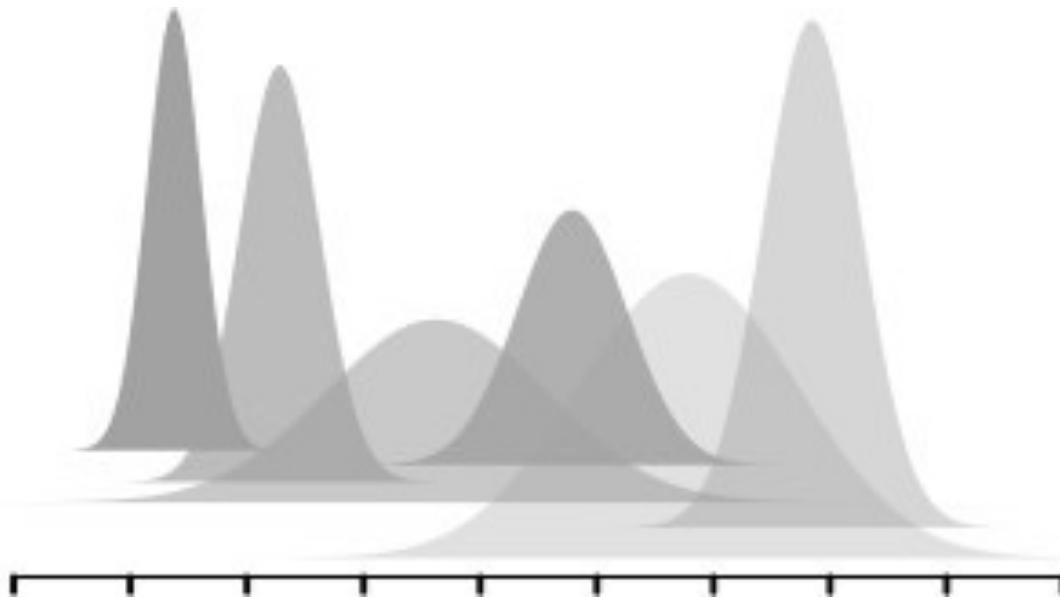


# 4.3 Fitting empirical data to models



Jelena H. Pantel

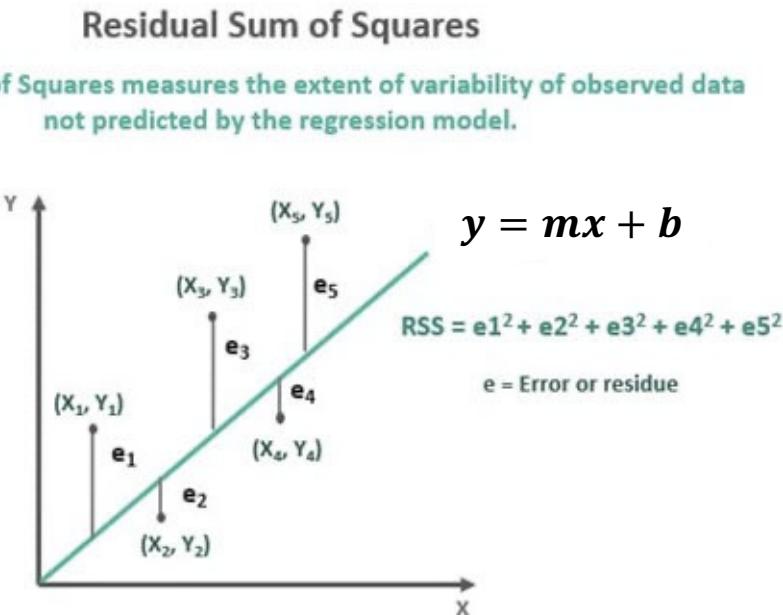
Faculty of Biology

University of Duisburg-Essen

jelena.pantel@uni-due.de

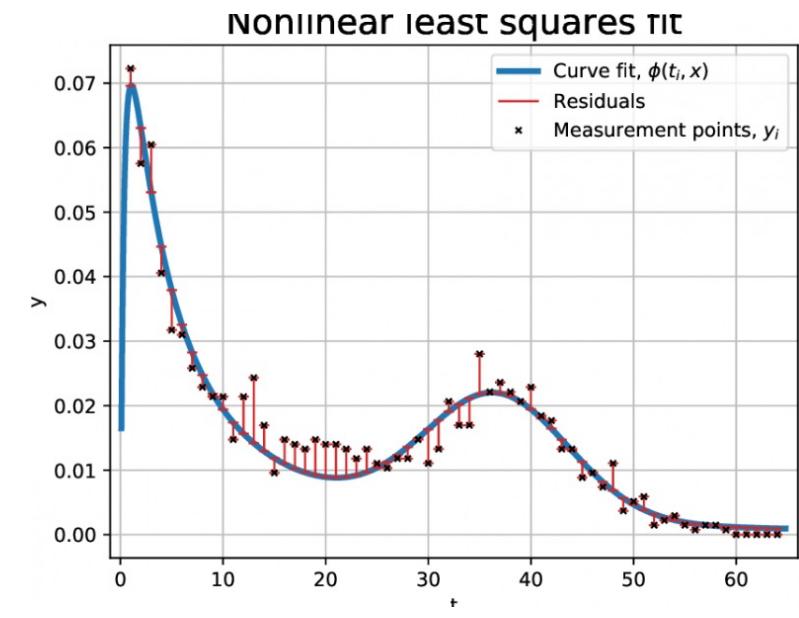
# Approaches to fit data to models

## Approach 1. Least squares and non-linear least squares

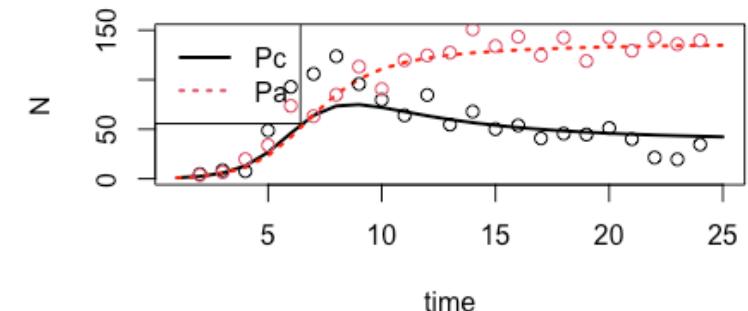


**Goal:** estimate parameters in linear or non-linear models by minimizing the residual sum of squares (RSS)

The smaller the RSS, the smaller the deviation between model-predicted line and observed data → the better the model fits the data



$$\frac{dn_i}{dt} = rn_i \left( 1 - \frac{n_i + \alpha_{ij}n_j}{K_i} \right)$$



# Approaches to fit data to models

Other approaches: Bayesian parameter estimation

What is the goal of these methods? To estimate the *most likely value* of the model parameters, given the data

We present this as – we want to know the *likelihood of the model parameter values given the data*

What is the probability of the model parameter value  $\Phi$   
Given the observed data  $y$

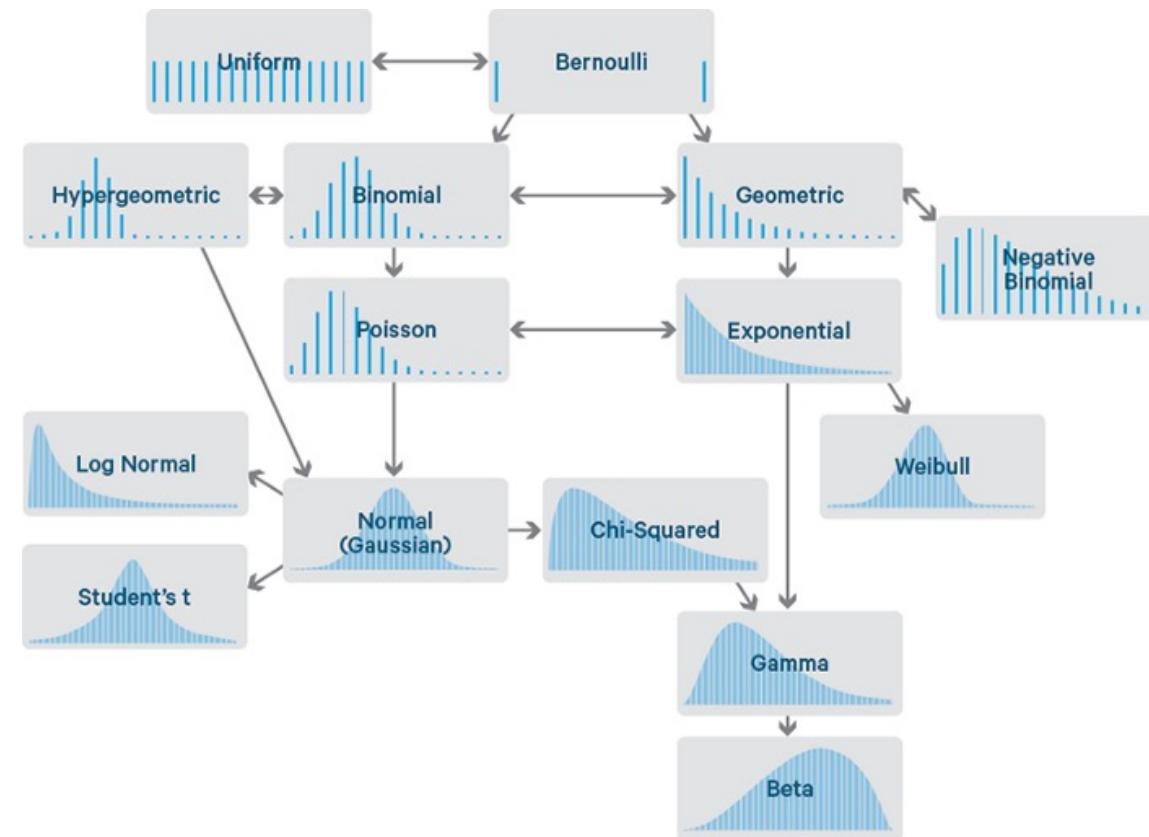
In a Bayesian framework, we (1) propose a *prior distribution* for each model parameter  $\Phi$

$$\frac{dn_i}{dt} = rn_i \left(1 - \frac{n_i + \alpha_{ij}n_j}{K_i}\right)$$

$\Phi = r, \alpha, K$

- What is the possible ranges of the parameter? – positive, negative, minimum, maximum?
- Continuous, discrete?

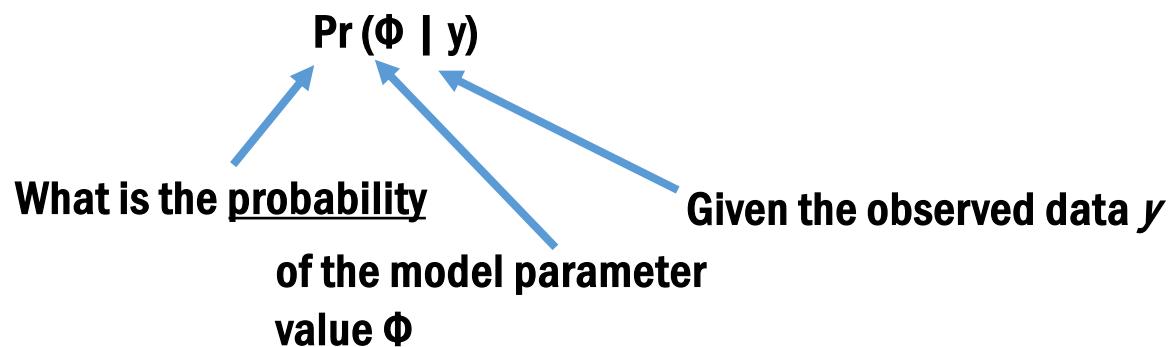
Possible probability distributions to choose from for model parameters



# Approaches to fit data to models

Other approaches: Bayesian parameter estimation

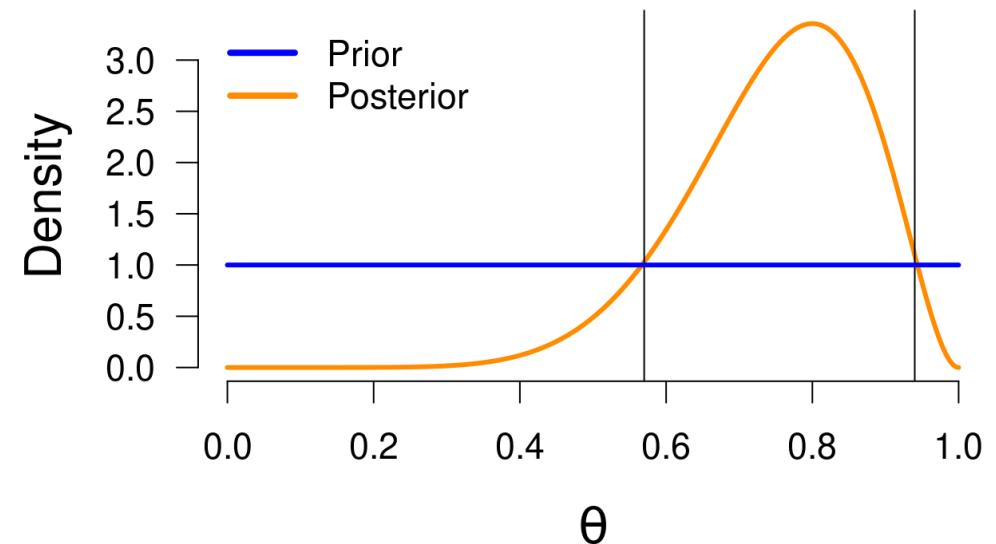
(1) In a Bayesian framework, we propose a prior distribution for each model parameter  $\Phi$



(2) Our goal is to:

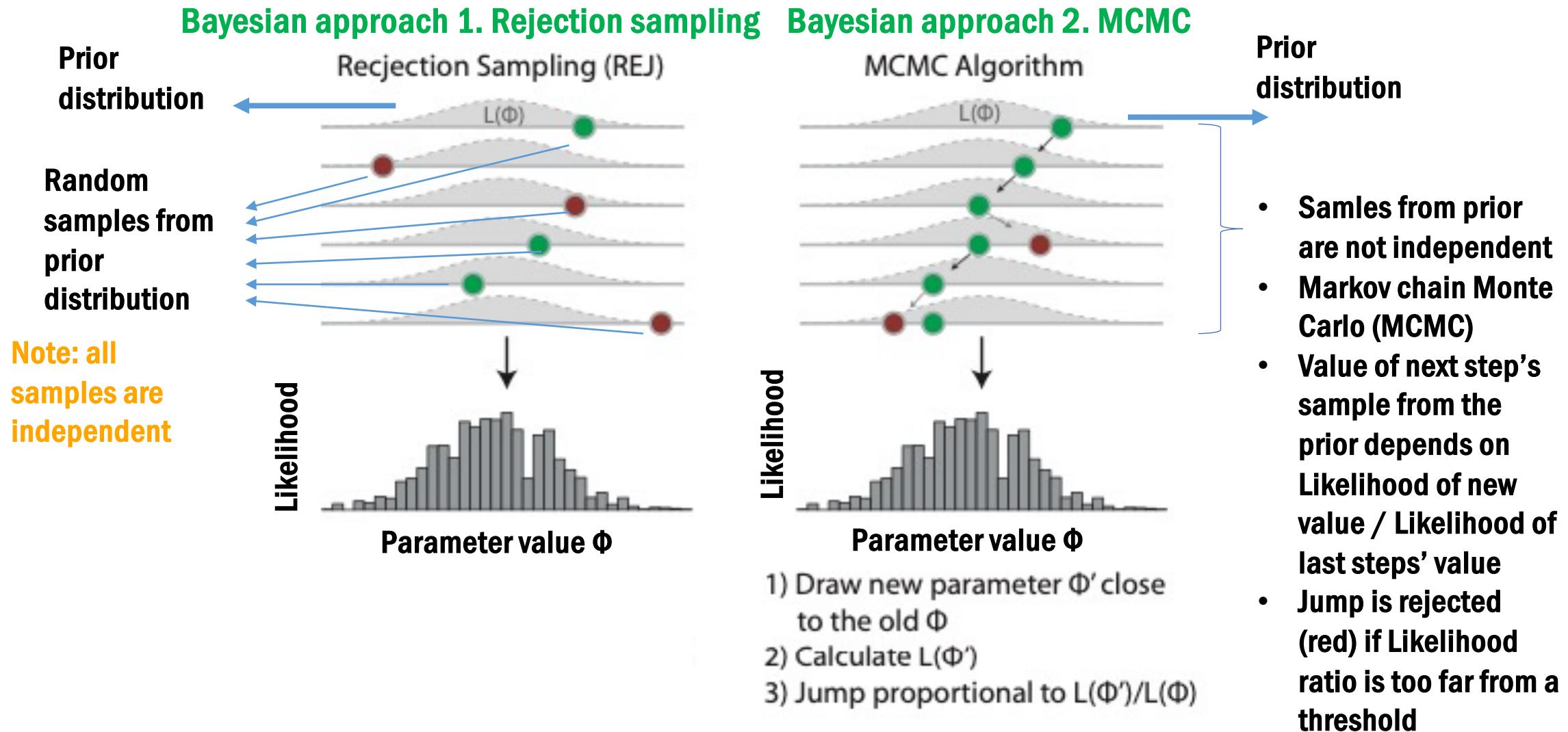
- propose different possible values of the parameters  $\Phi$  (using the prior distribution)
- calculate the likelihood those being the ‘true’ parameter values given the data  $\Pr (\Phi | y)$
- Find the posterior distribution of parameters, based on the likelihood calculations above

In other words, we use some kind of *likelihood* value to go from a prior distribution to a posterior distribution of model parameters



# Approaches to fit data to models

Other approaches: Bayesian parameter estimation



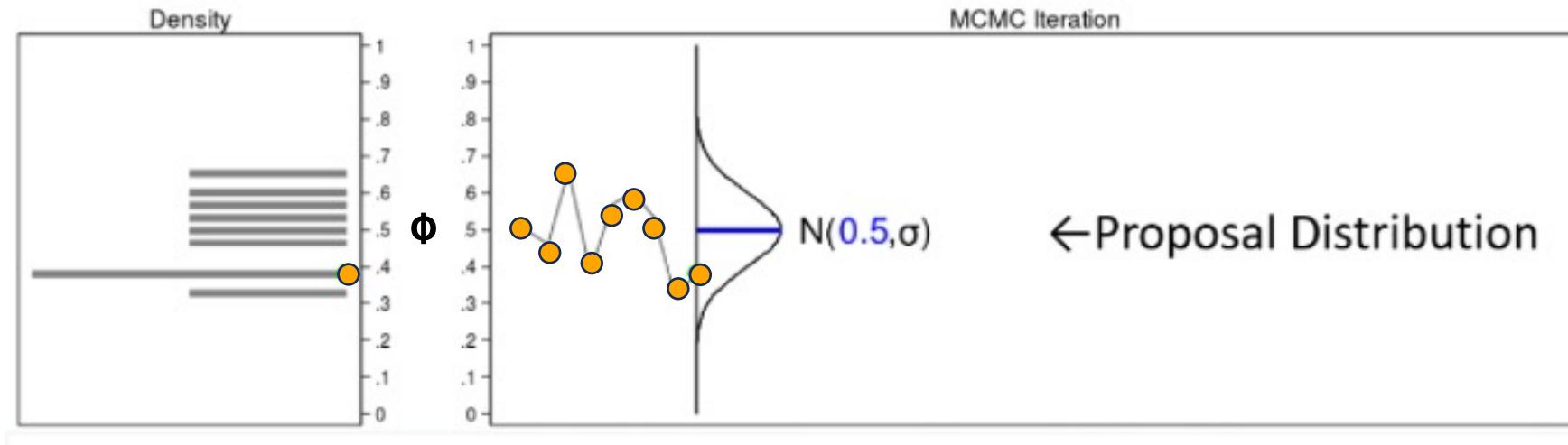
# Approaches to fit data to models

## Approach 2. Bayesian MCMC

Example: Estimate the mean of a normal distribution using MCMC

In this example, the true value  $\Phi = 0.5$

Figure 1: Proposal distributions, trace plots, and density plots



# Approaches to fit data to models

## Approach 2. Bayesian MCMC

Example: Estimate the mean of a normal distribution using MCMC

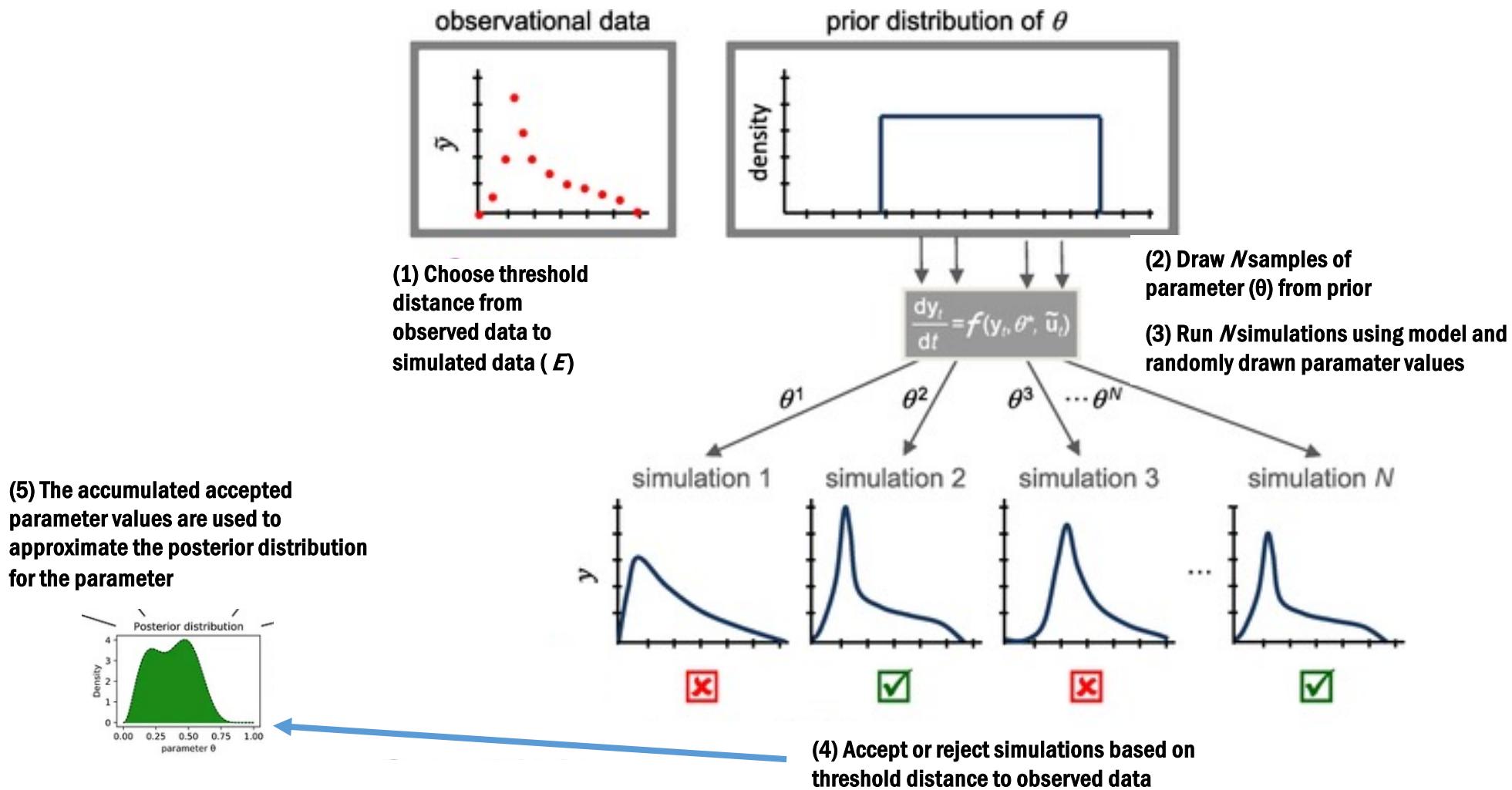
In this example, the true value  $\Phi = 0.5$



Draw  $\theta_t \sim \text{Normal}(0.5, \sigma) = 0.460$

# Approaches to fit data to models

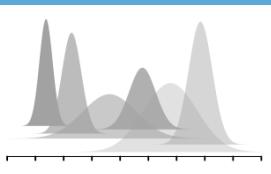
## Approach 3. Approximate Bayesian computation (ABC)



# Eco-evolutionary dynamics – overlapping ecological and evolutionary processes that are not independent of one another



Gil Garcia, <https://www.flickr.com/photos/giltastic/7219581854/>



# Research approach – eco-evolutionary hypothesis testing to fit data to models



Candidate model

1. Identify candidate models for processes that structure observed data

Ecoevo  
 $H_0, H_A$

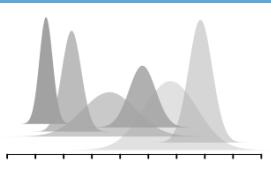
2. Generate alternative eco-evolutionary hypotheses

Simulations

3. Simulate possible observed data under each hypothesis

Compare to  
observed data

4. Compare observed data to alternative hypothesis simulations



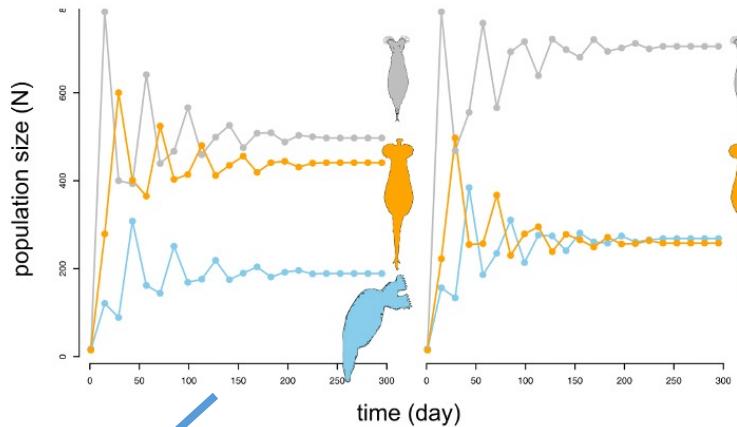
# Research approach – eco-evolutionary hypothesis testing to fit data to models



Candidate model

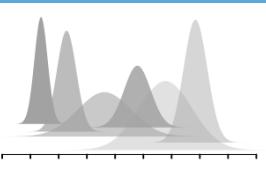
1. Identify candidate models for processes that structure observed data

Ex 1) Coexistence / competition for a few species



$$\frac{N_{i,t+1}}{N_{i,t}} = \frac{\lambda_i(x)}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}}$$

growth rate (as a function of a trait  $x$ )  
Intraspecific competition rate    Interspecific competition rate



# Research approach – eco-evolutionary hypothesis testing to fit data to models

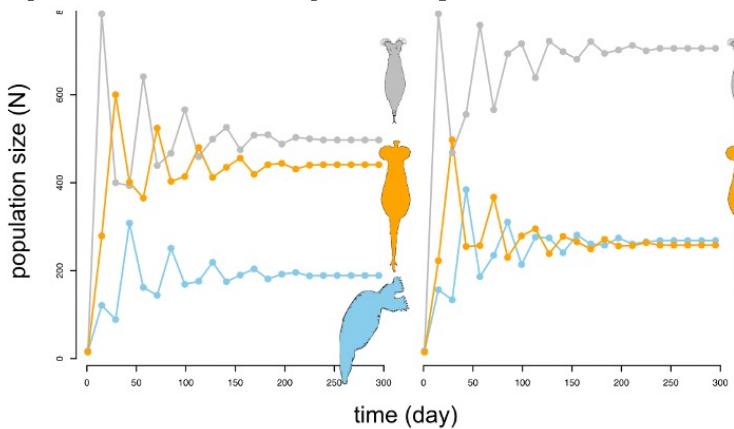


Ecoevo  
 $H_0, H_A$

Simulations

2. Generate alternative eco-evolutionary hypotheses
3. Simulate possible observed data under each hypothesis

## Ex 1) Coexistence / competition for a few species



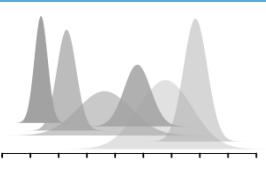
$H_{\text{eco}}$

Trait  $x$  does not evolve

$H_{\text{eco-evo}}$

Trait  $x$  can evolve

$$\frac{N_{i,t+1}}{N_{i,t}} = \frac{\lambda_i(x)}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}}$$



# Research approach – eco-evolutionary hypothesis testing to fit data to models

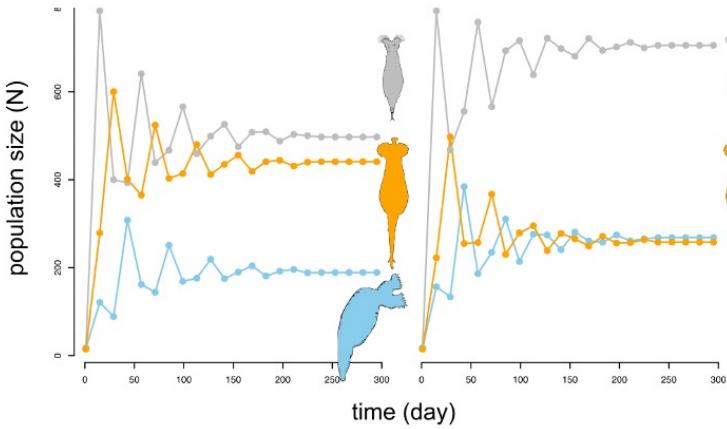


Ecoevo  
 $H_0, H_A$

Simulations

2. Generate alternative eco-evolutionary hypotheses
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## Ex 1) Coexistence / competition for a few species



$H_{\text{eco}}$   
Trait  $x$  does not evolve

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Trait  $x$  can evolve

$$\frac{N_{i,t+1}}{N_{i,t}} = \frac{\lambda_i(x)}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}}$$

$$\lambda_t = \bar{W}_t = \widehat{We}^{-\frac{[(w+(1-h^2)P)(E-x_t)]^2}{2(P+w)}}$$

width of phenotypic distribution

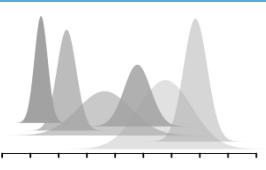
strength of selection

heritability of trait  $x$

Distance between trait  $x$  and optimum trait value  $E$

Growth rate  
→ fitness

$$\lambda_t = \bar{W}_t = \widehat{We}$$



# Research approach – eco-evolutionary hypothesis testing to fit data to models

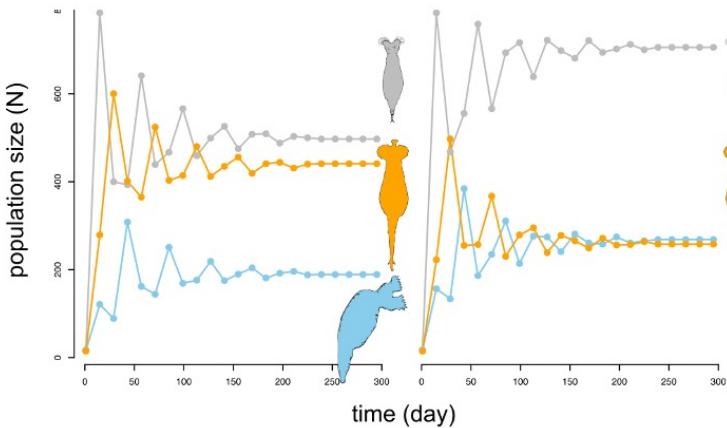


Ecoevo  
 $H_0, H_A$

Simulations

2. Generate alternative eco-evolutionary hypotheses
3. Simulate possible observed data under each hypothesis

## Ex 1) Coexistence / competition for a few species



$H_{\text{eco}}$   
Trait  $x$  does not evolve

$$\frac{N_{i,t+1}}{N_{i,t}} = \frac{\lambda_i(x)}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}}$$

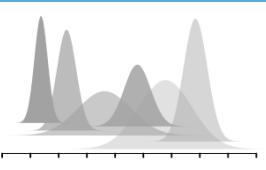
$H_{\text{eco-evo}}$   
Trait  $x$  can evolve

Growth rate  
→ fitness

$$\lambda_t = \bar{W}_t = \hat{W} e^{-\left[\left(\frac{(w+(1-h^2)P)}{P+w}\right)(E-x_t)\right]^2}$$

$$N_{i,t+1} = \frac{\hat{W} e^{-\left[\left(\frac{(w+(1-h^2)P)}{P+w}\right)(E-x_t)\right]^2}}{1 + \alpha_{ii}N_{i,t} + \sum_j \alpha_{ij}N_{j,t}} N_{i,t}$$

width of phenotypic distribution  
strength of selection  
heritability of trait  $x$   
Distance between trait  $x$  and optimum trait value  $E$



# Research approach – eco-evolutionary hypothesis testing to fit data to models

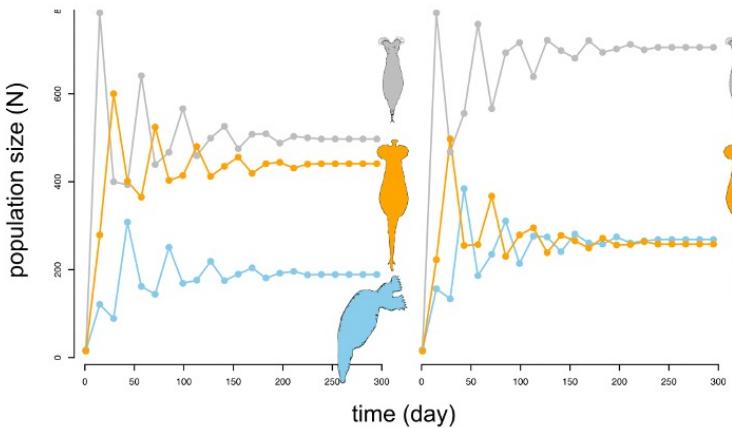


Ecoevo  
 $H_0, H_A$

Simulations

2. Generate alternative eco-evolutionary hypotheses
3. Simulate possible observed data under each hypothesis

## Ex 1) Coexistence / competition for a few species



$H_{\text{eco}}$

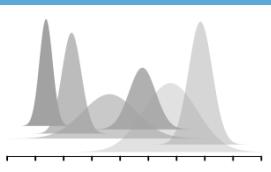
Trait  $x$  does not evolve

$$\frac{N_{i,t+1}}{N_{i,t}} = \frac{\lambda_i(x)}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}}$$

$H_{\text{eco-evo}}$

Trait  $x$  can evolve

$$N_{i,t+1} = \frac{\hat{W} e^{-[(\frac{w+(1-h^2)P}{P+w})(E-x_t)]^2}}{1 + \alpha_{ii}N_{i,t} + \sum_j \alpha_{ij}N_{j,t}} N_{i,t}$$



# Research approach – eco-evolutionary hypothesis testing to fit data to models



Simulations

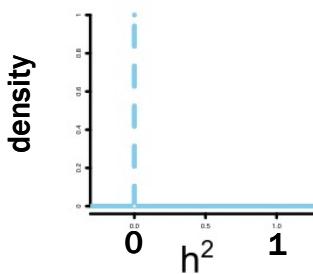
Compare to observed data

3. Simulate possible observed data under each hypothesis

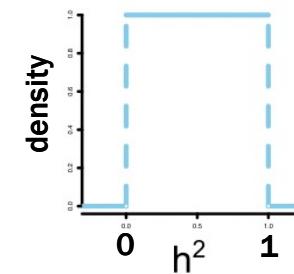
4. Compare observed data to alternative hypothesis simulations

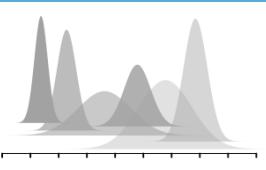
sample a candidate parameter vector  $\theta^*$  from a proposed prior distribution, 100,000 simulations per model

$H_1$ : No evolution ( $h^2=0$ )



$H_2$ : Evolution ( $h^2>0$ )





# Research approach – eco-evolutionary hypothesis testing to fit data to models



Simulations

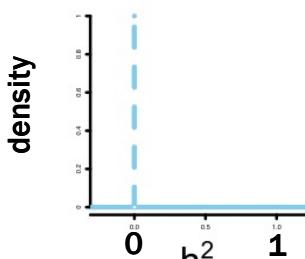
Compare to observed data

3. Simulate possible observed data under each hypothesis

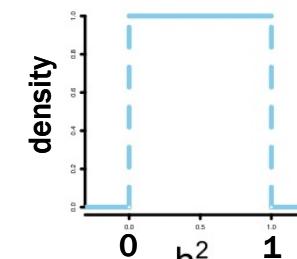
4. Compare observed data to alternative hypothesis simulations

sample a candidate parameter vector  $\theta^*$  from a proposed prior distribution, 100,000 simulations per model

$H_1$ : No evolution ( $h^2=0$ )

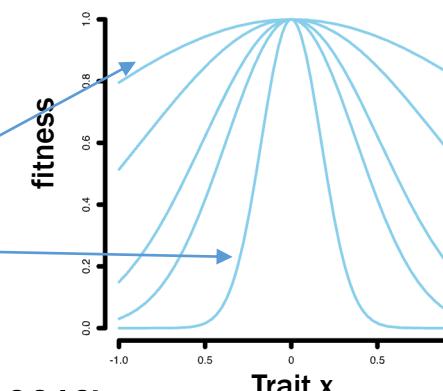
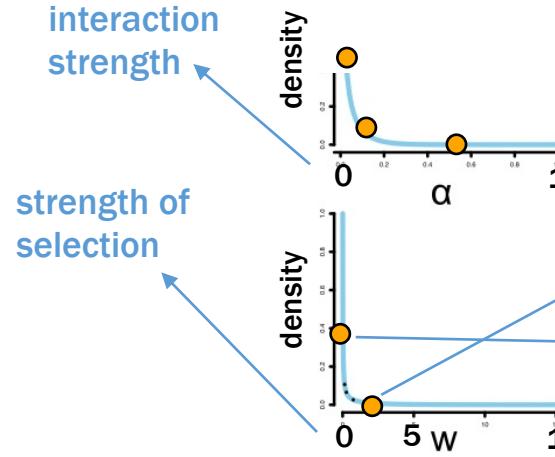


$H_2$ : Evolution ( $h^2>0$ )



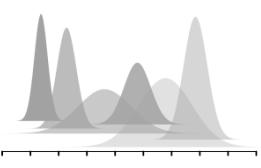
interaction strength

strength of selection



Approximate Bayesian Computing (eg Beaumont 2010)

Model parameters:  $h^2, \alpha, w, \widehat{W}, P$



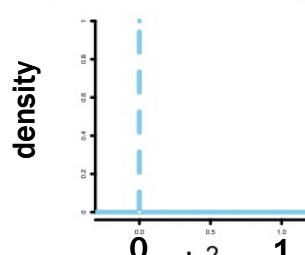
# Research approach - eco-evolutionary hypothesis testing to fit data to models



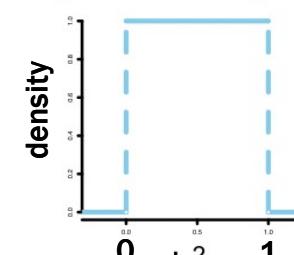
Simulations

Compare to observed data

$H_1$ : No evolution ( $h^2=0$ )

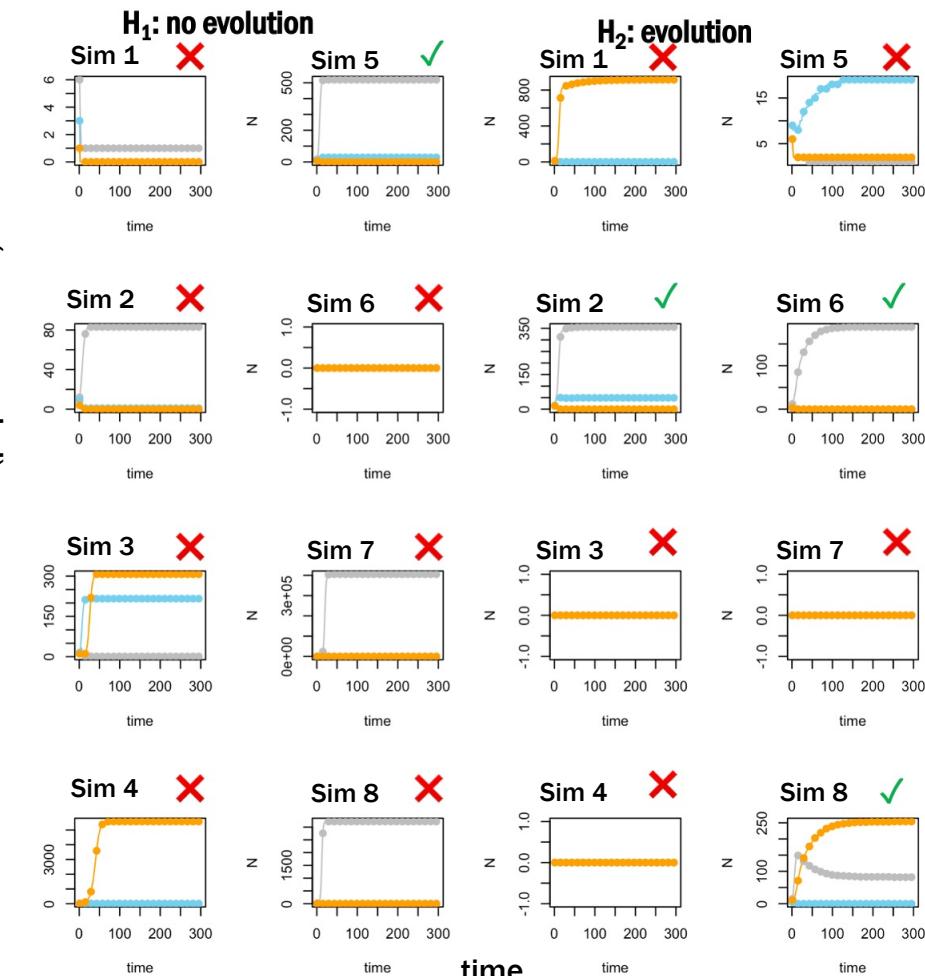
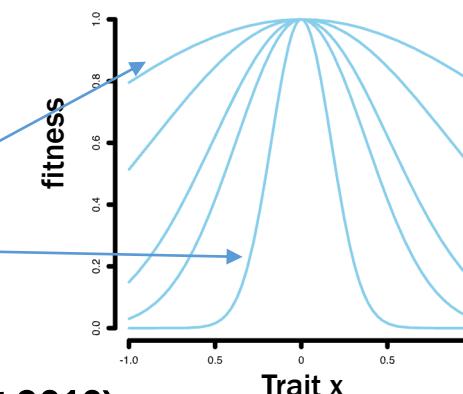
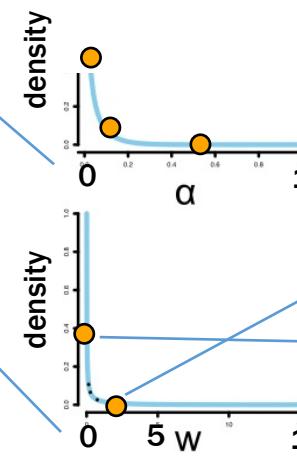


$H_2$ : Evolution ( $h^2>0$ )



interaction strength

strength of selection

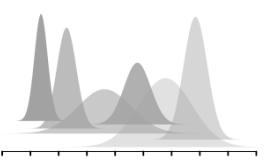


sample a candidate parameter vector  $\theta^*$  from a proposed prior distribution, 100,000 simulations per model

compare the simulated dataset  $x^*$  to the observed data  $x_0$ , using a distance function  $d$  and a tolerance  $\varepsilon$ : if  $d(x_0, x^*) \leq \varepsilon$ , accept  $\theta^*$

Approximate Bayesian Computing (eg Beaumont 2010)

Model parameters:  $h^2, \alpha, w, \widehat{W}, P$



# Research approach - eco-evolutionary hypothesis testing to fit data to models



Compare to observed data

## 4. Compare observed data to alternative hypothesis simulations

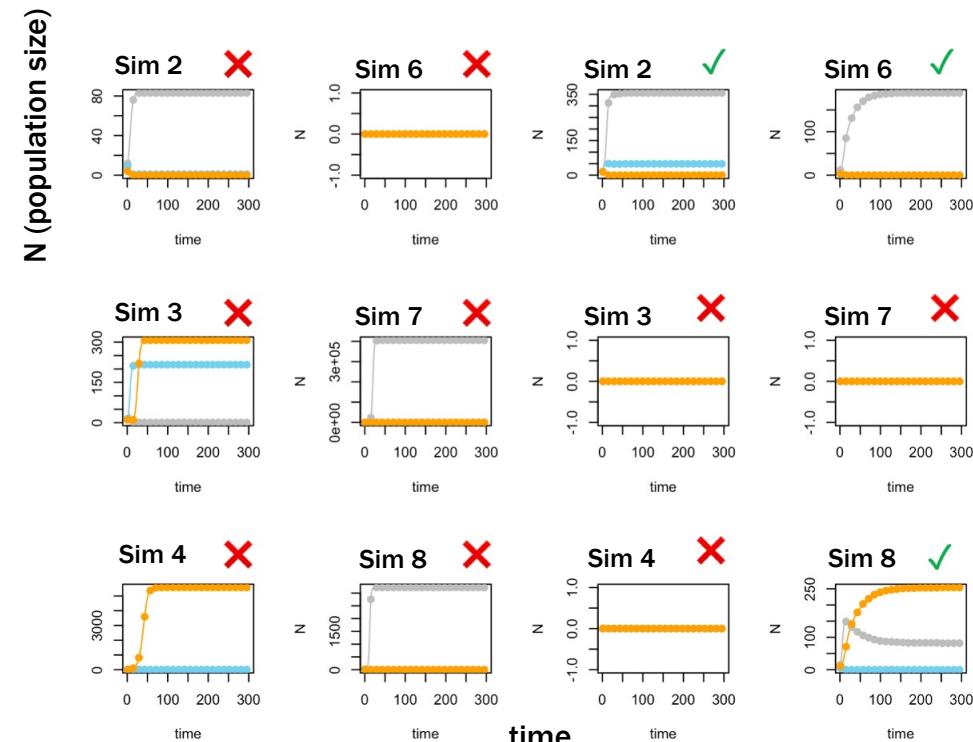
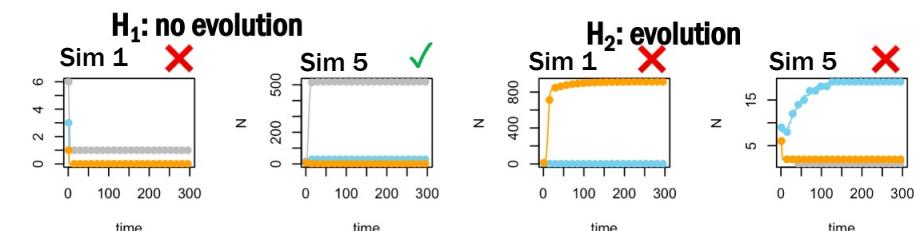
### (i) Estimate posterior probability of alternative model hypotheses

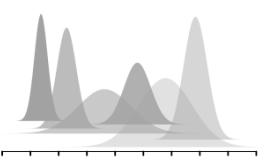
$H_{\text{eco}}$

$$\frac{n_{i,t+1}}{n_{i,t}} = \frac{\lambda_i}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}}$$

$H_{\text{eco-evo}}$

$$N_{i,t+1} = \hat{W}e^{\frac{-[(\frac{w+(1-h^2)P}{P+w})(E-x_t)]^2}{2(P+w)}} N_{i,t}$$





# Research approach - eco-evolutionary hypothesis testing to fit data to models



Compare to observed data

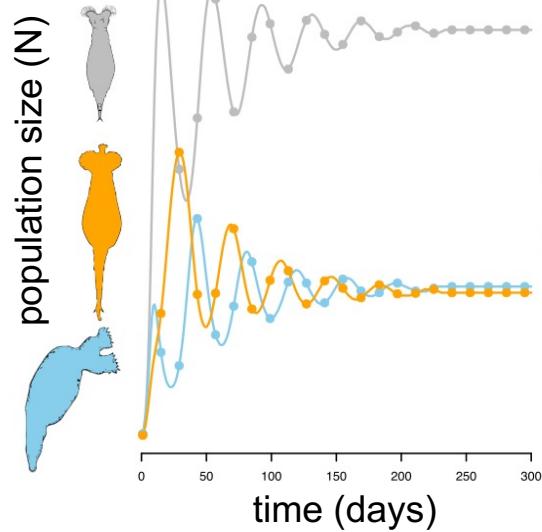
## 4. Compare observed data to alternative hypothesis simulations

### (i) Estimate posterior probability of alternative model hypotheses

$$\begin{aligned} H_{\text{eco}} & \\ \frac{n_{i,t+1}}{n_{i,t}} &= \frac{\lambda_i}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}} \quad H_{\text{eco-evo}} = \frac{\hat{W}e^{-\frac{[(\frac{w+(1-h^2)P}{P+w})(E-x_t)]^2}{2(P+w)}}}{1 + \alpha_{ii}N_{i,t} + \sum_j \alpha_{ij}N_{j,t}} N_{i,t} \end{aligned}$$

Case 1. With simulated model + data

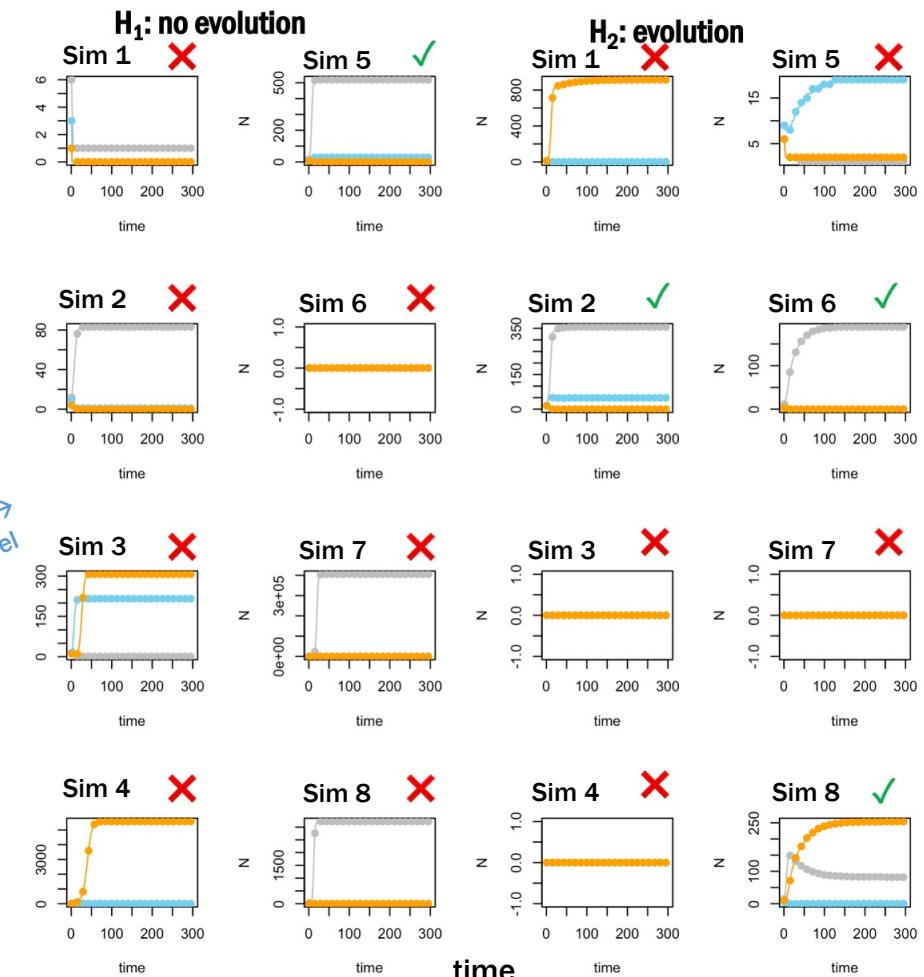
With  $x_0$  and  $x_{300}$  trait values

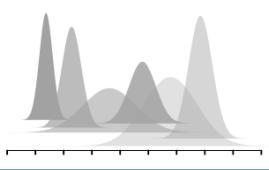


Posterior model probabilities for Observed Data

$$\begin{aligned} H_{\text{eco}} &= 0.0001 \\ H_{\text{eco-evo}} &= 0.9999 \end{aligned}$$

Based on % Accepted vs. Rejected per  $H_A$  model  
Approximate Bayesian Computing + Neural network (for model classification) → trained on 100,000 simulations per model





# Research approach – eco-evolutionary hypothesis testing to fit data to models



## Compare to observed data

#### **4. Compare observed data to alternative hypothesis simulations**

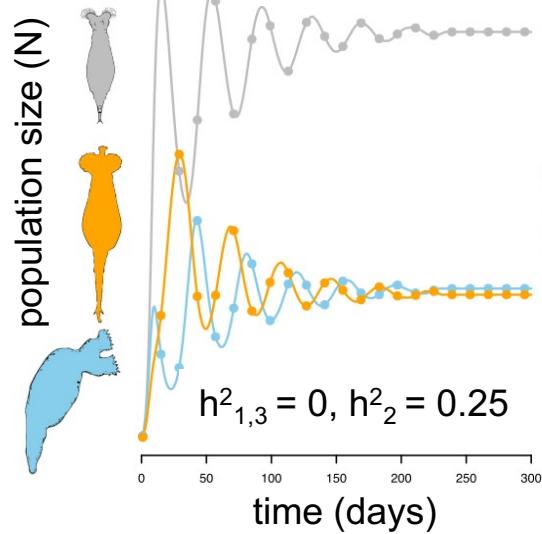
(i) Estimate posterior probability of alternative model hypotheses

$$\frac{n_{i,t+1}}{n_{i,t}} = \frac{\lambda_i}{1 + \alpha_{ii}N_{i,t} + \alpha_{ij}N_{j,t}} \quad N_{i,t+1}$$

$$H_{\text{eco-evo}} \quad N_{i,t+1} = \frac{\hat{We}^{\frac{-[(\frac{w+(1-h^2)P}{P+w})(E-x_t)]^2}{2(P+w)}} N_{i,t}}{1 + \alpha_{ii}N_{i,t} + \sum_j \alpha_{ij}N_{j,t}}$$

## Case 1. With simulated model + data

## With $x_0$ and $x_{300}$ trait values



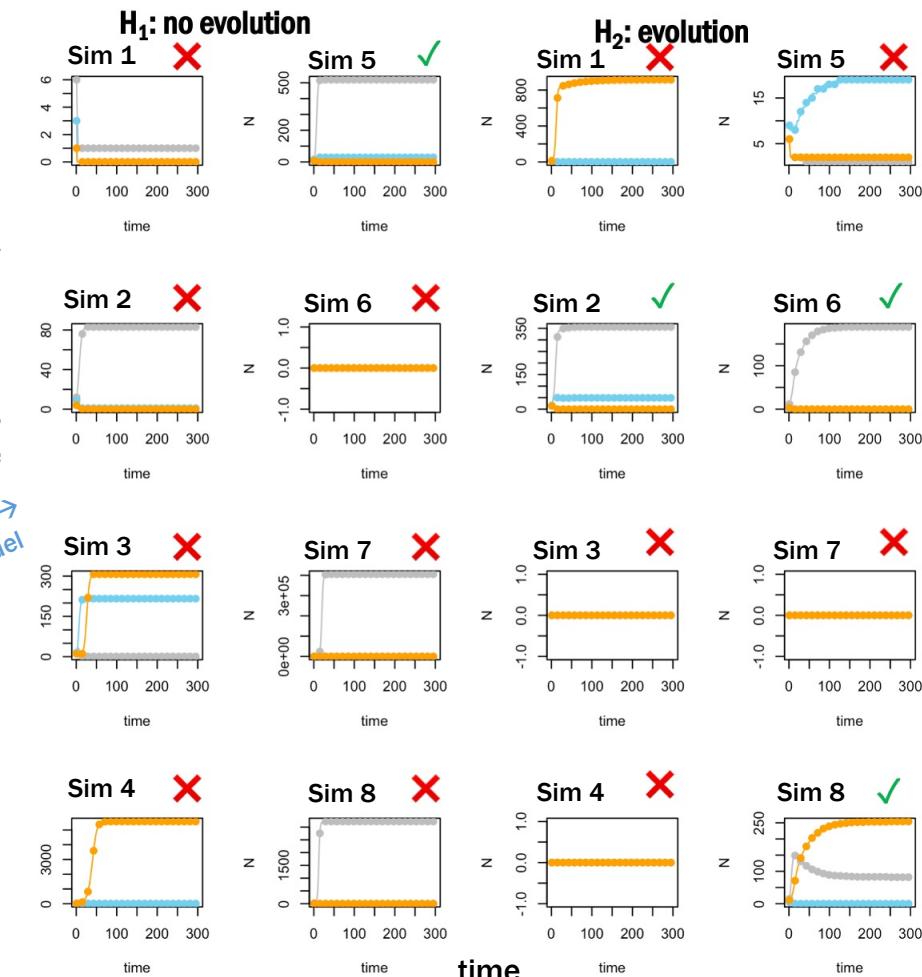
## Posterior model probabilities for Observed Data

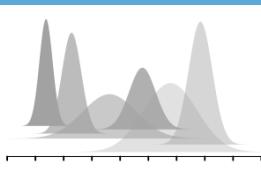
$$H_{\text{eco}} = 0.0001 \quad \times$$
$$H_{\text{eco-evo}} = 0.9999 \quad \checkmark$$

Approximate Bayesian Computing +  
Neural network (for model classification)  
trained on 100,000 simulations per mode

Based on % Accepted vs.  
Rejected per  $H_A$  model

$N$  (populations)





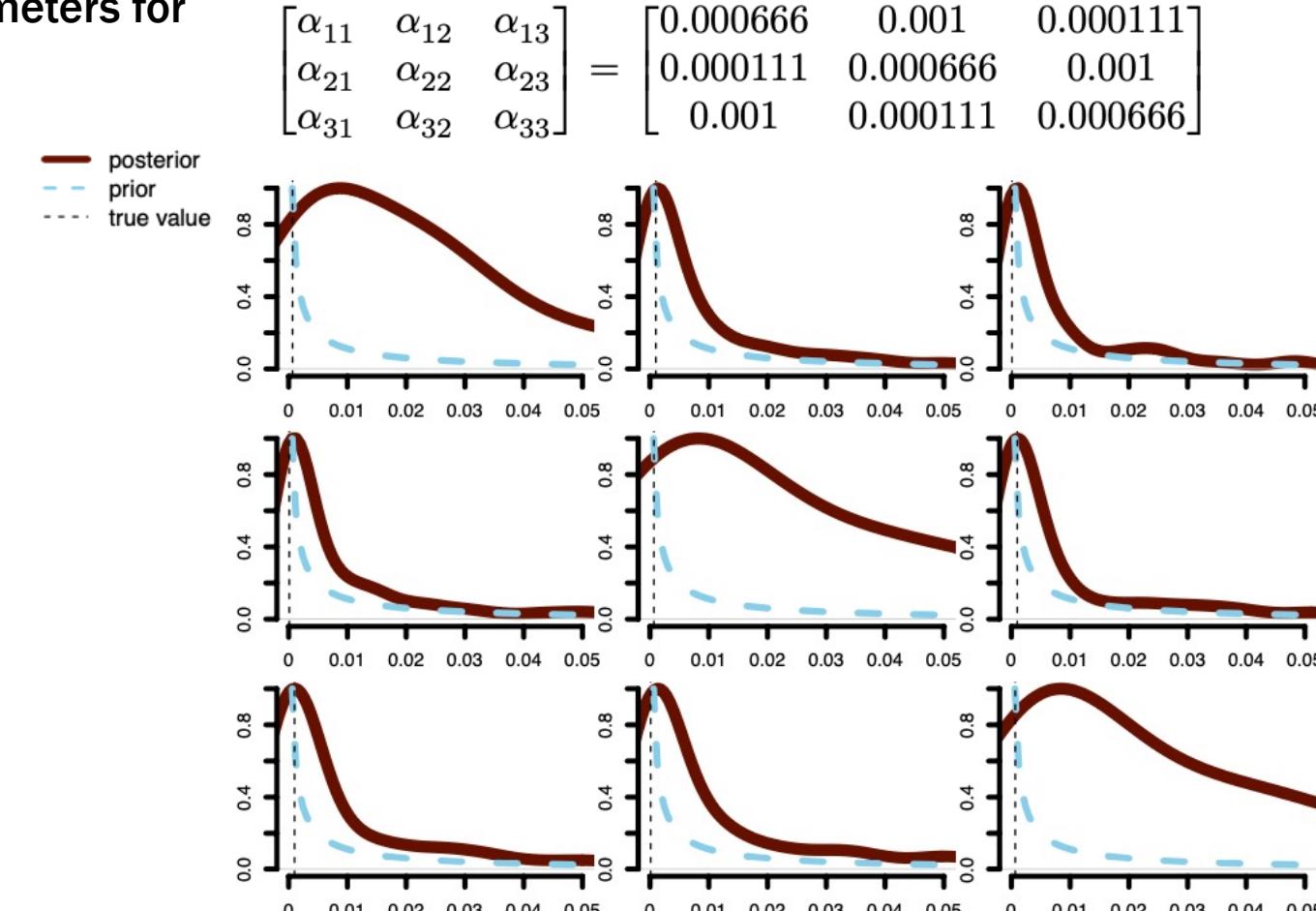
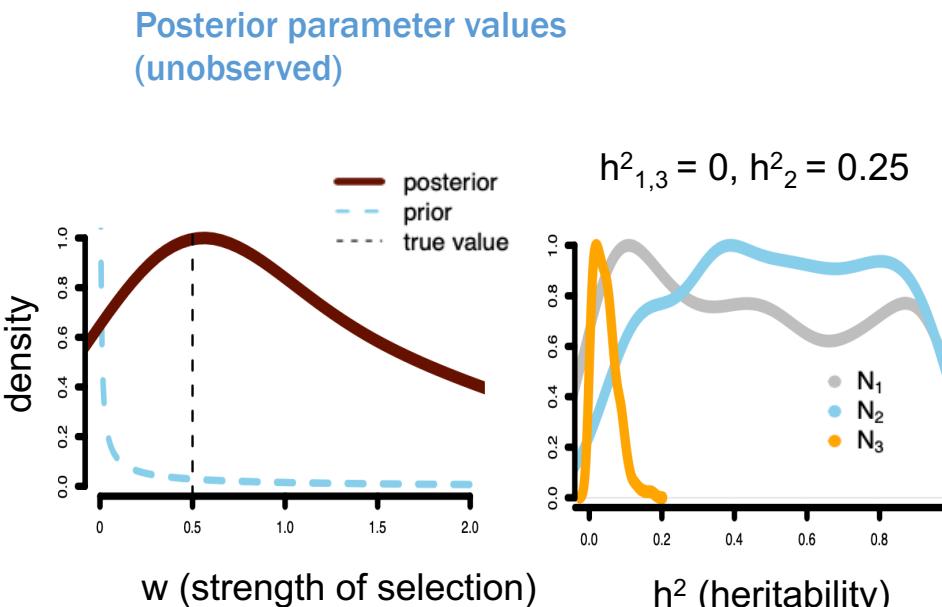
# Research approach – eco-evolutionary hypothesis testing to fit data to models

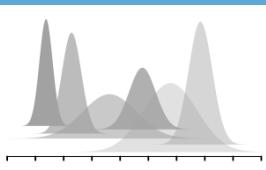


Compare to observed data

## 4. Compare observed data to alternative hypothesis simulations

- (i) Estimate posterior probability of alternative model hypotheses
- (ii) Use best-fit (or consensus) models to estimate parameters for observed data, make predictions for future cases





# Research approach – eco-evolutionary hypothesis testing to fit data to models



Compare to observed data

## 4. Compare observed data to alternative hypothesis simulations

- (i) Estimate posterior probability of alternative model hypotheses
- (ii) Use best-fit (or consensus) models to estimate parameters for observed data, make predictions for future cases

