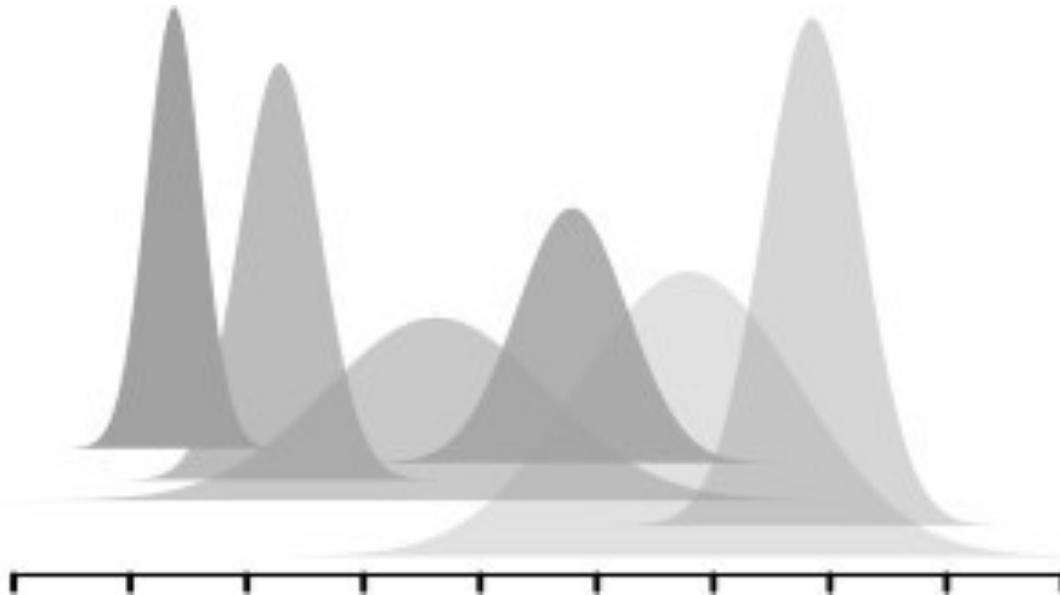


4.3 Fitting empirical data to models



Jelena H. Pantel

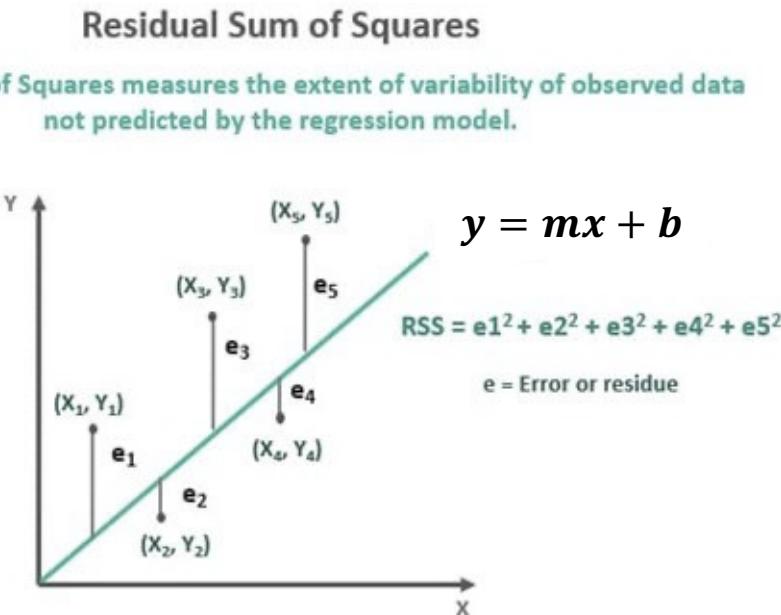
Faculty of Biology

University of Duisburg-Essen

jelena.pantel@uni-due.de

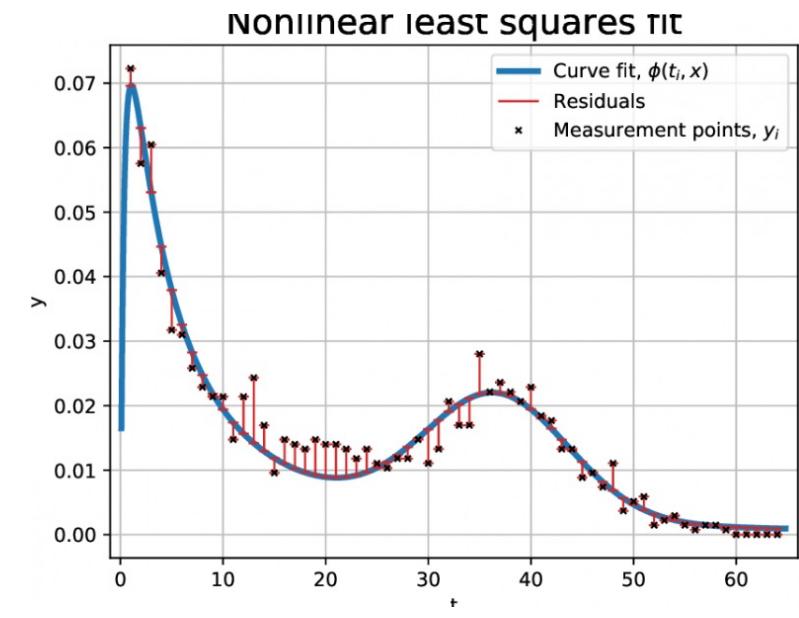
Approaches to fit data to models

Approach 1. Least squares and non-linear least squares

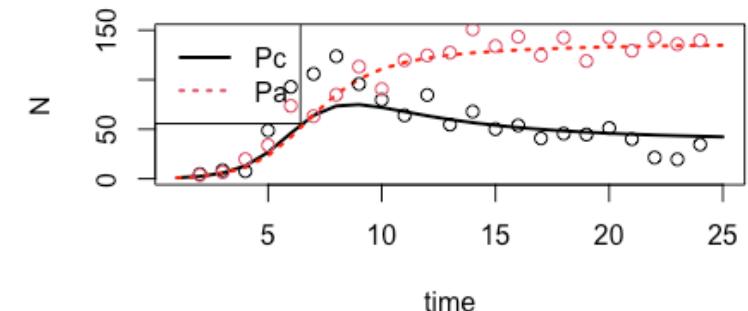


Goal: estimate parameters in linear or non-linear models by minimizing the residual sum of squares (RSS)

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 Φ
Given the observed data y

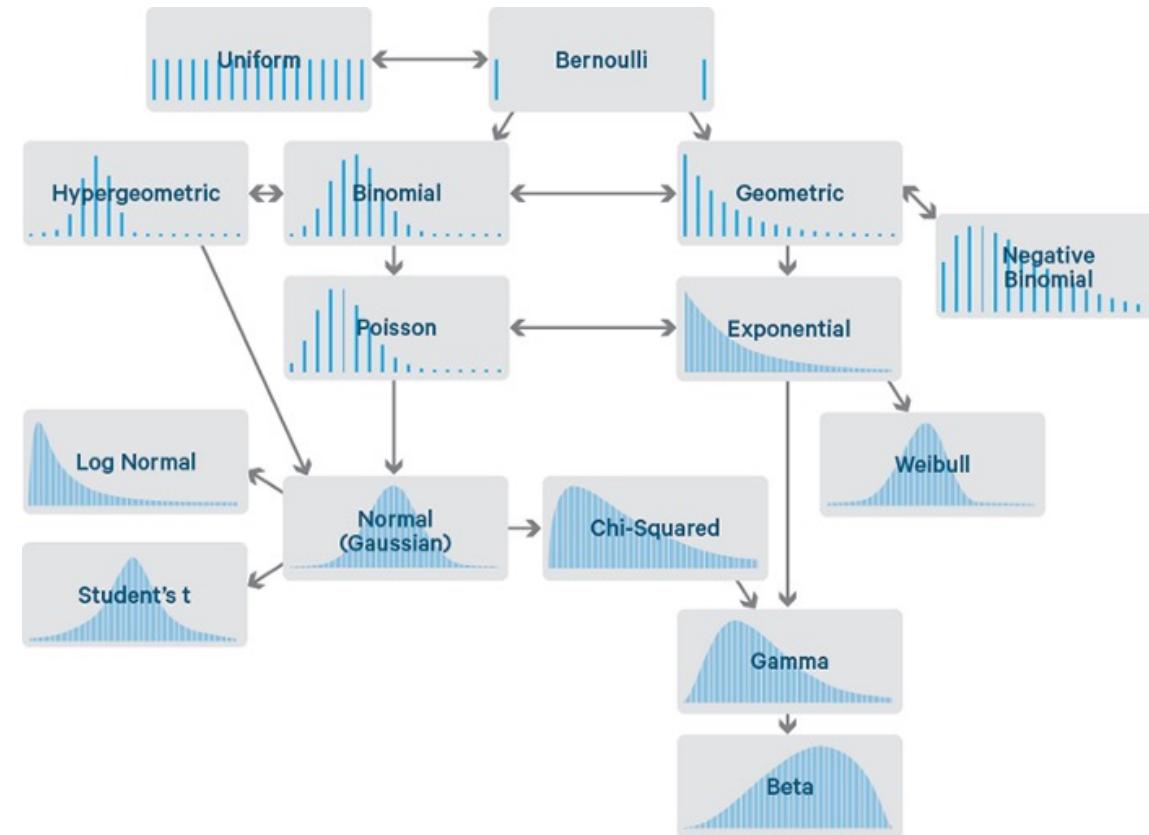
In a Bayesian framework, we (1) propose a *prior distribution* for each model parameter Φ

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

$\Phi = r, \alpha, K$

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

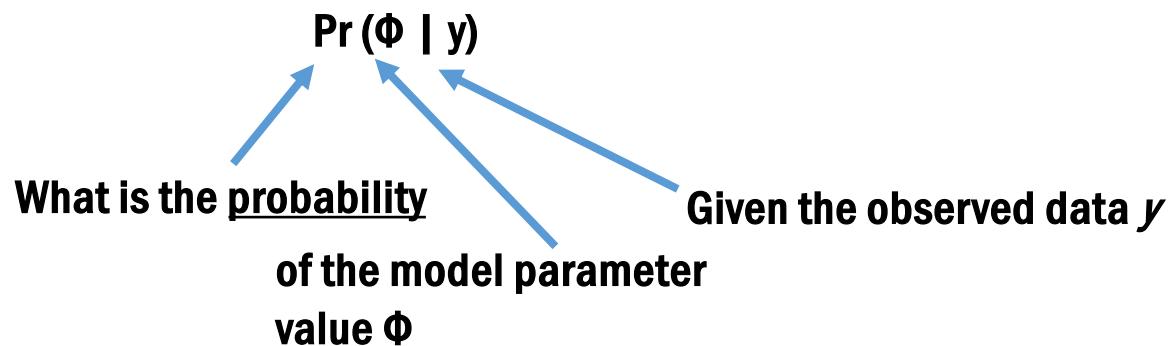
Possible probability distributions to choose from for model parameters



Approaches to fit data to models

Other approaches: Bayesian parameter estimation

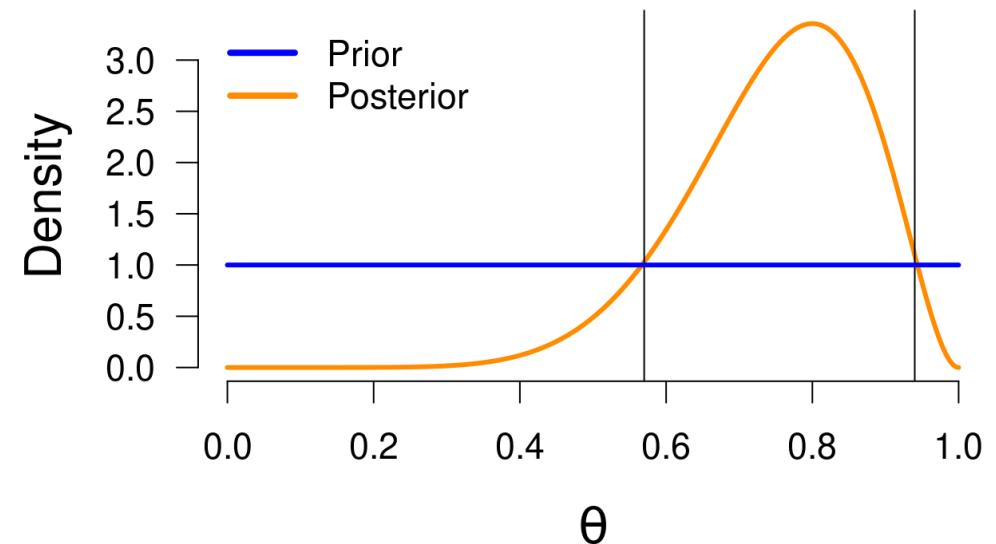
(1) In a Bayesian framework, we propose a prior distribution for each model parameter Φ



(2) Our goal is to:

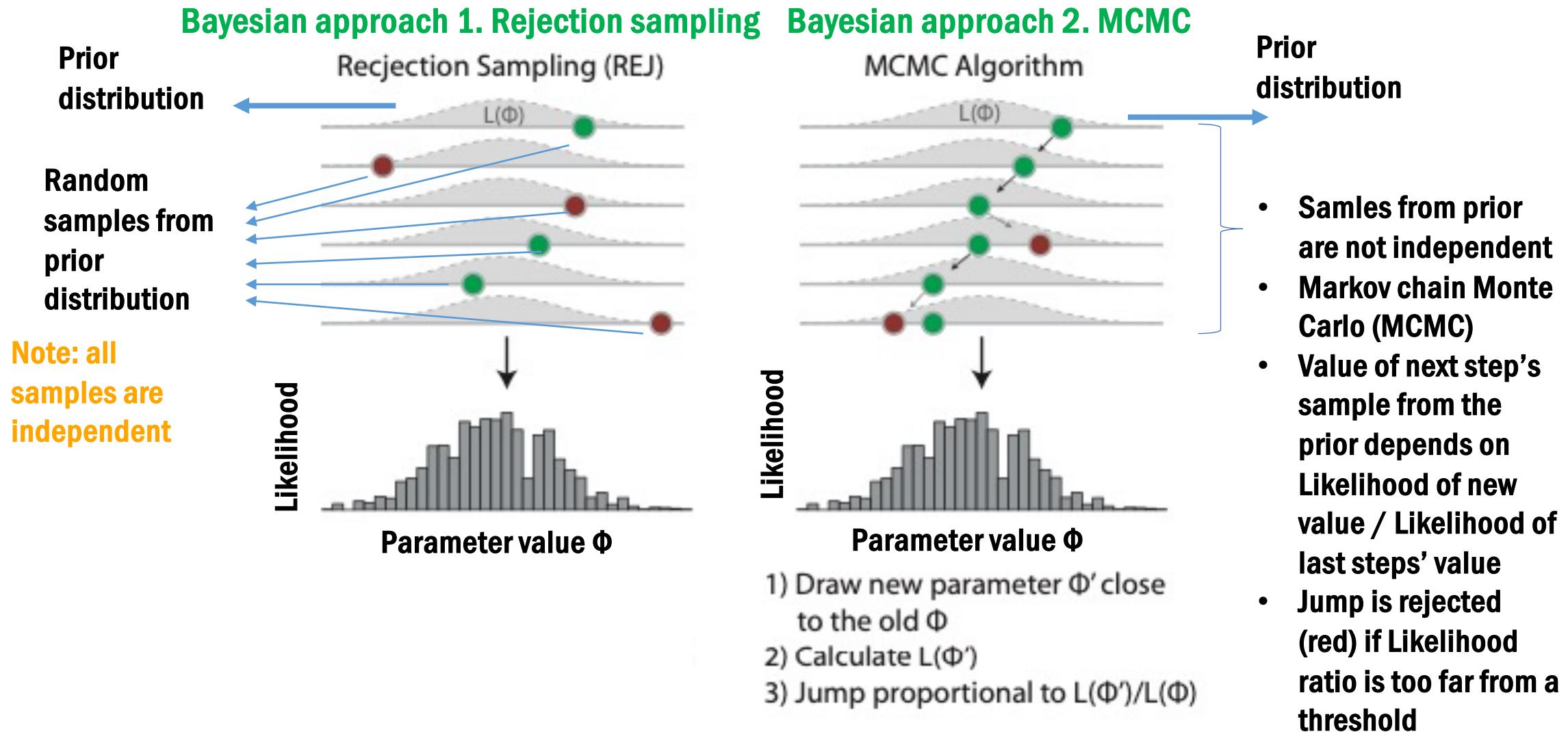
- propose different possible values of the parameters Φ (using the prior distribution)
- calculate the likelihood those being the ‘true’ parameter values given the data $\Pr (\Phi | y)$
- Find the posterior distribution of parameters, based on the likelihood calculations above

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



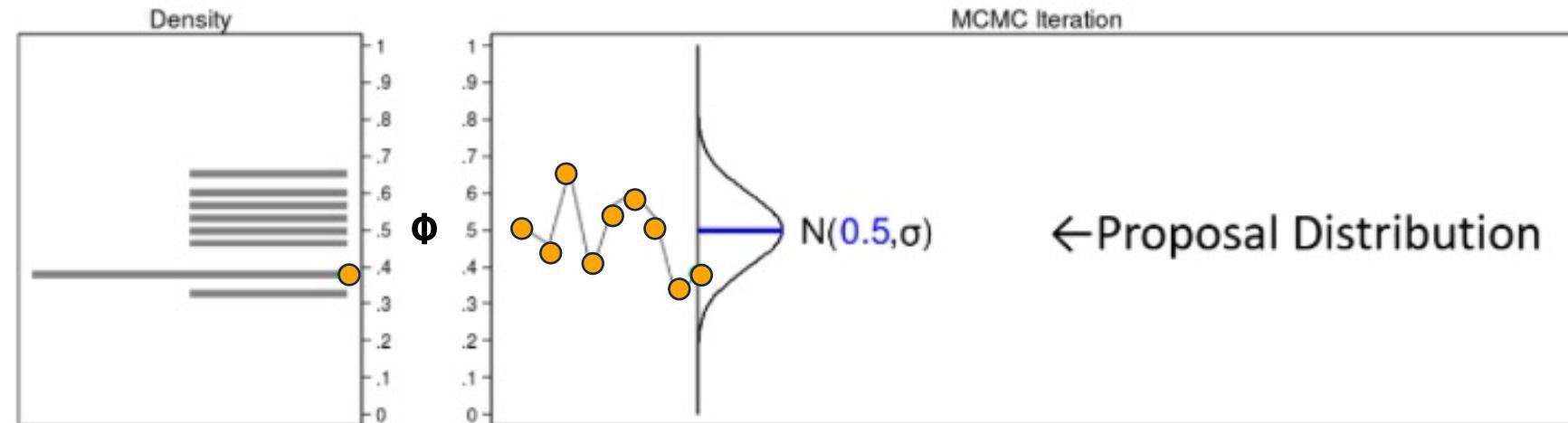
Approaches to fit data to models

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



←Proposal Distribution



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

Approaches to fit data to models

Approach 2. Bayesian MCMC

Example: Estimate the mean of a normal distribution using MCMC

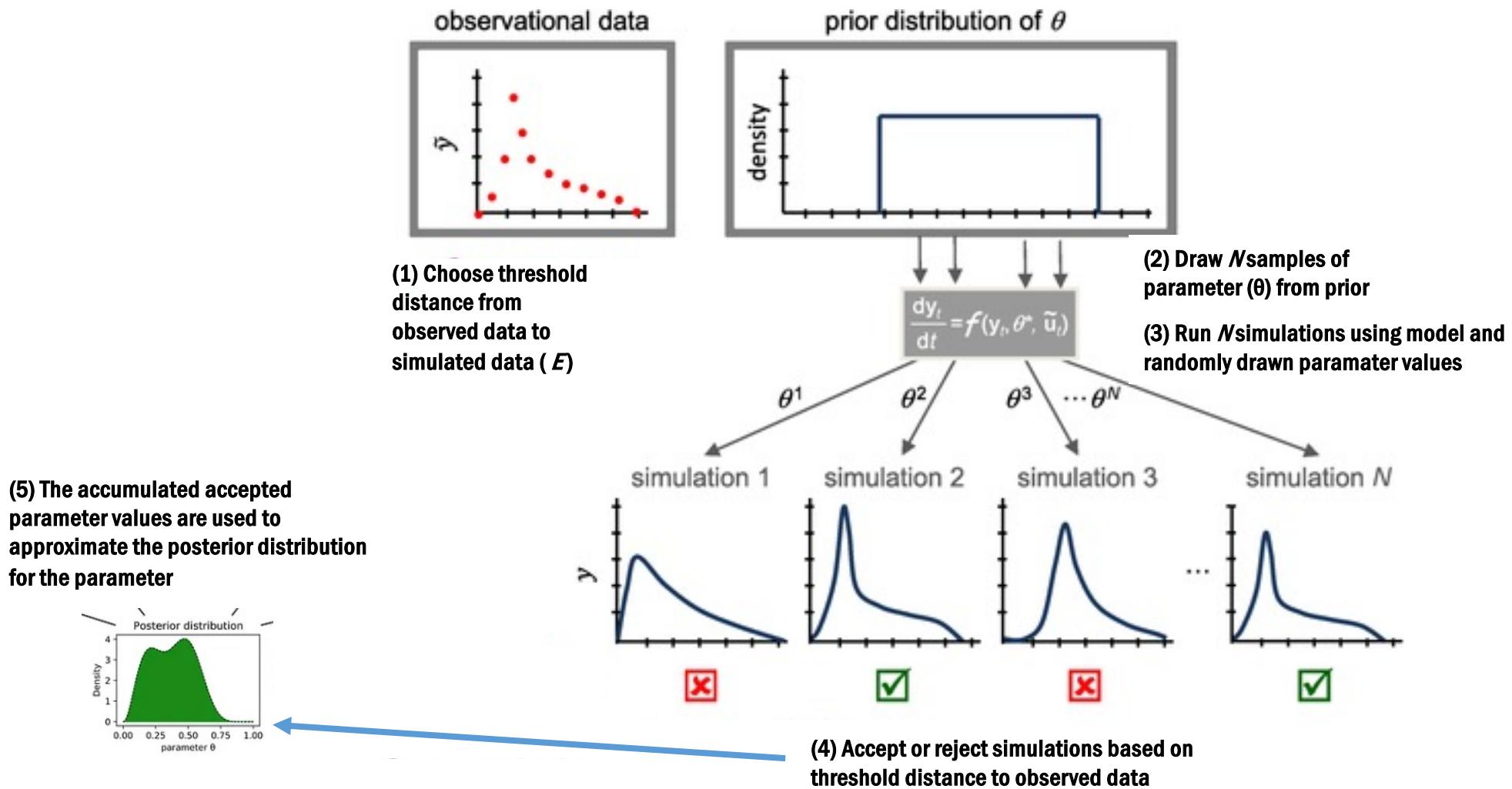
In this example, the true value $\Phi = 0.5$

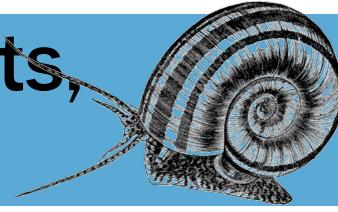


Draw $\theta_t \sim \text{Normal}(0.5, \sigma) = 0.460$

Approaches to fit data to models

Approach 3. Approximate Bayesian computation (ABC)

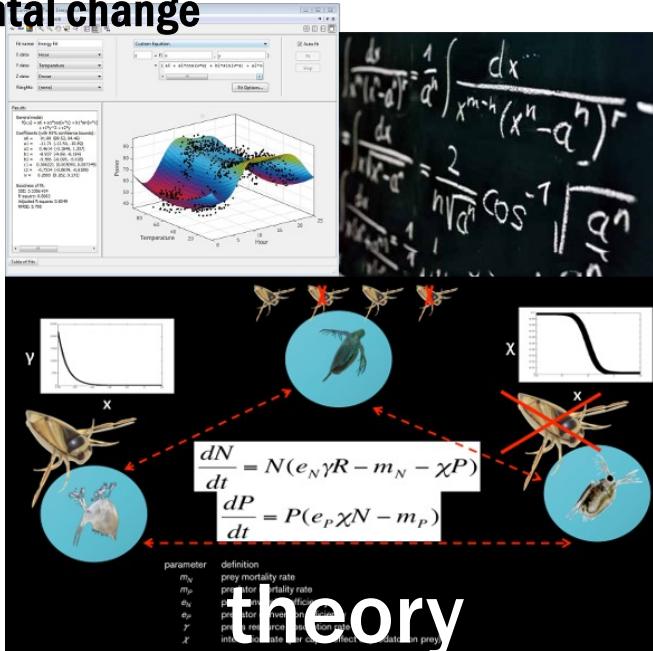




Research approach – combine surveys, experiments, and models

Research goals

- Develop accurate models to explain and predict biodiversity
- Understand the consequences of evolution for communities, metacommunities, and ecosystems
- Determine how eco-evolutionary dynamics influence the response of biodiversity to environmental change

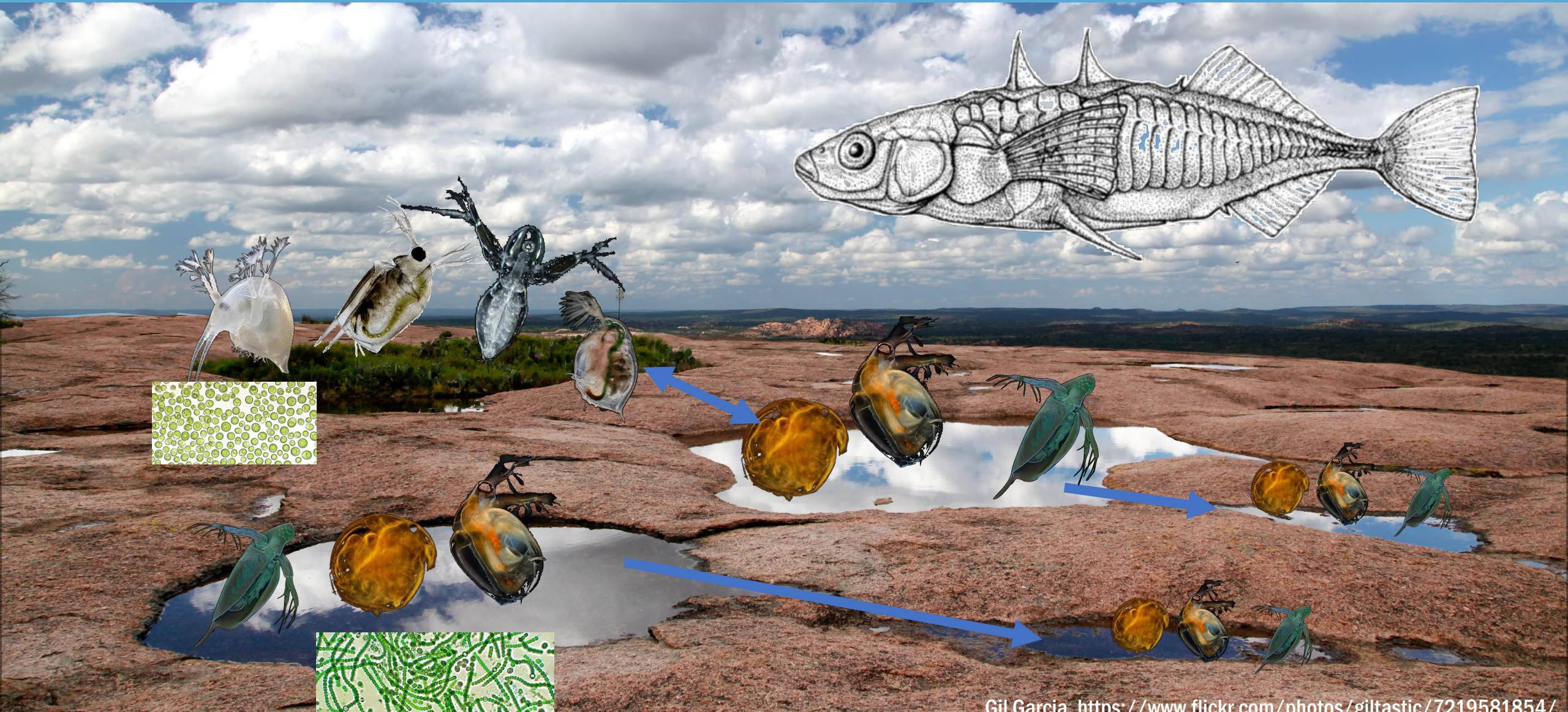


experiment



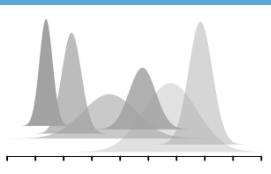
observation

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



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





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

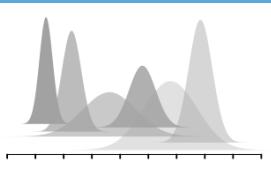
2. Generate alternative eco-evolutionary hypotheses

Simulations

3. Simulate possible observed data under each hypothesis

Compare to
observed data

4. Compare observed data to alternative hypothesis simulations



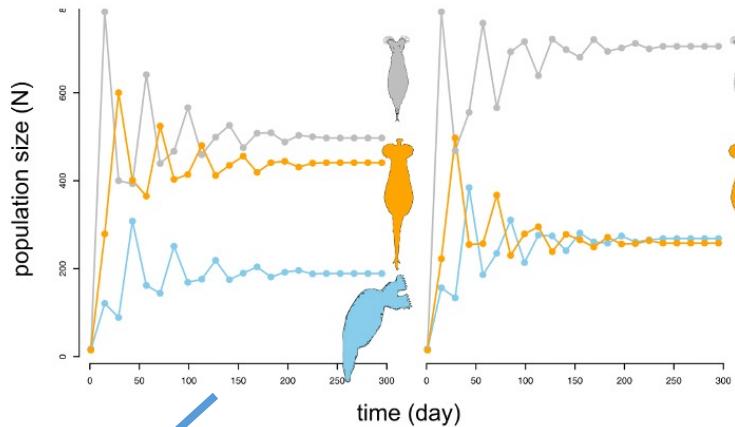
Research approach – eco-evolutionary hypothesis testing to fit data to models



Candidate model

1. Identify candidate models for processes that structure observed data

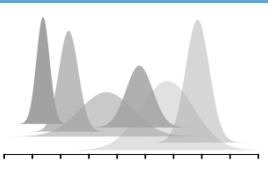
Ex 1) Coexistence / competition for a few species



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

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

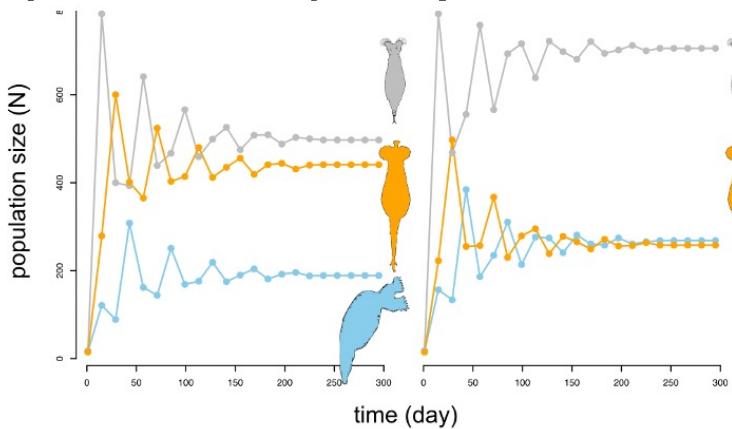


Ecoevo
 H_0, H_A

Simulations

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

Ex 1) Coexistence / competition for a few species



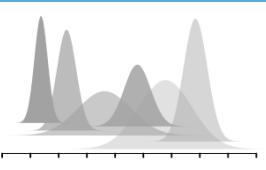
H_{eco}

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



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

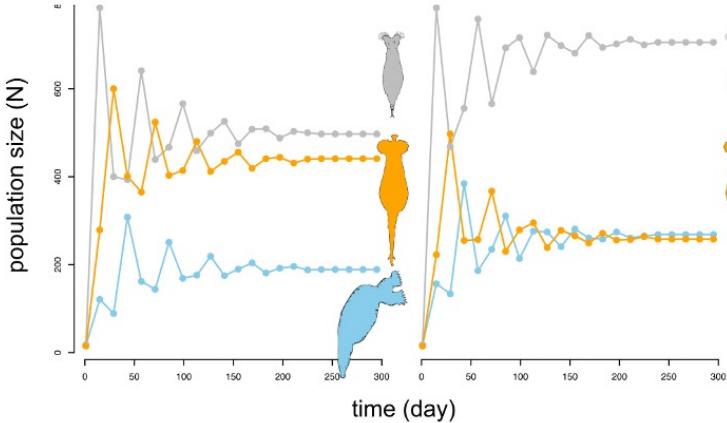


Ecoevo
 H_0, H_A

Simulations

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3. Simulate possible observed data under each hypothesis

Ex 1) Coexistence / competition for a few species



H_{eco}

Trait x does not evolve

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

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

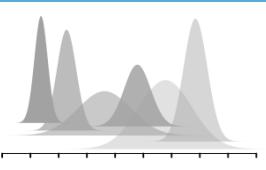
Trait x can evolve

Growth rate
→ fitness

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

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

$$-\left[\left(\frac{(w+(1-h^2)P)}{P+w}\right)(E-x_t)\right]^2$$



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

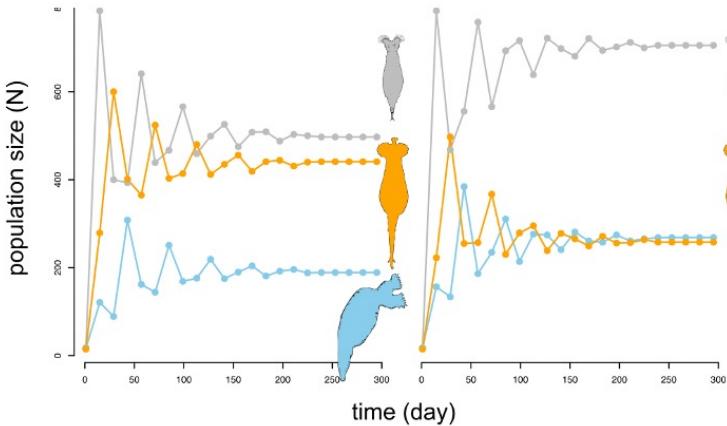


Ecoevo
 H_0, H_A

Simulations

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

Ex 1) Coexistence / competition for a few species



H_{eco}
Trait x does not evolve

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

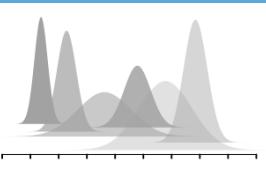
$H_{\text{eco-evo}}$
Trait x can evolve

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

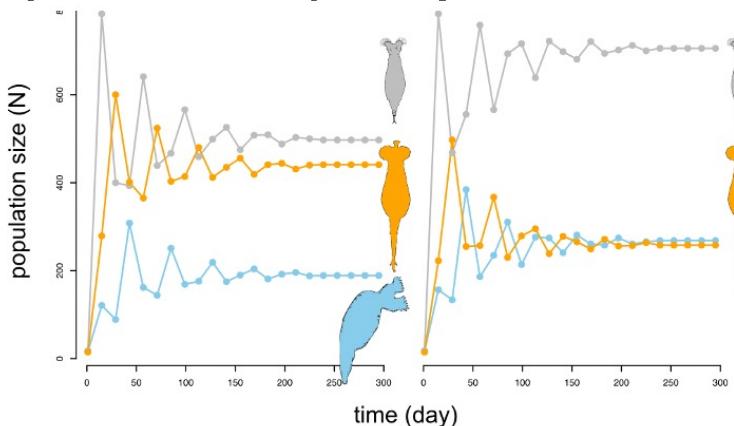


Ecoevo
 H_0, H_A

Simulations

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

Ex 1) Coexistence / competition for a few species



H_{eco}

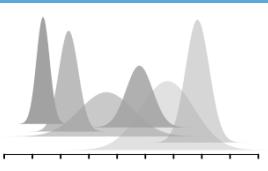
Trait x does not evolve

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

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

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

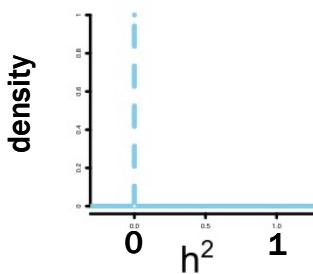
3. Simulate possible observed data under each hypothesis

Compare to observed data

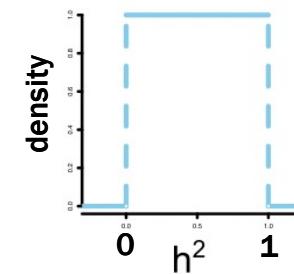
4. Compare observed data to alternative hypothesis simulations

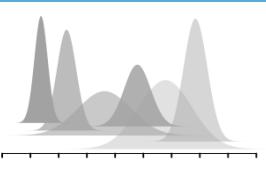
sample a candidate parameter vector θ^* from a proposed prior distribution, 100,000 simulations per model

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

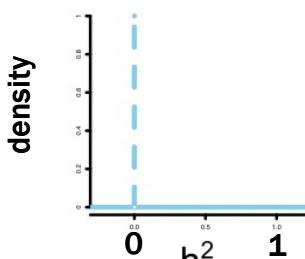
Compare to observed data

3. Simulate possible observed data under each hypothesis

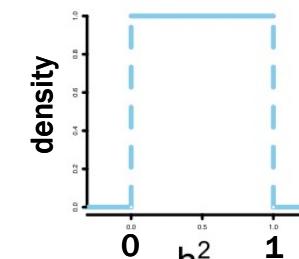
4. Compare observed data to alternative hypothesis simulations

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

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

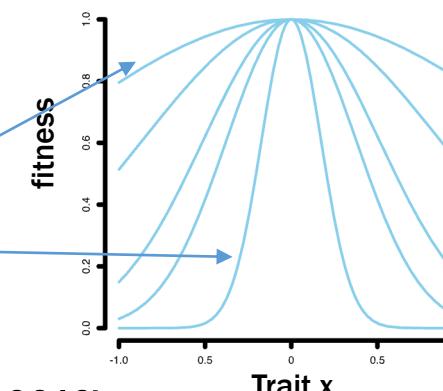
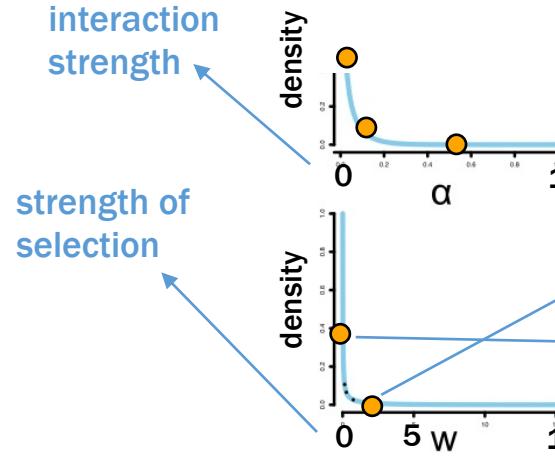


H_2 : Evolution ($h^2>0$)



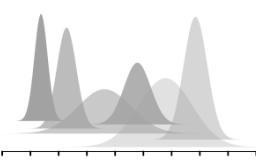
interaction strength

strength of selection



Approximate Bayesian Computing (eg Beaumont 2010)

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



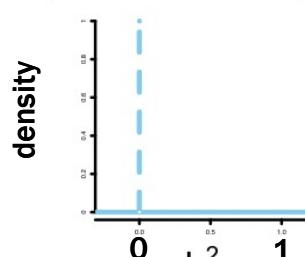
Research approach - eco-evolutionary hypothesis testing to fit data to models



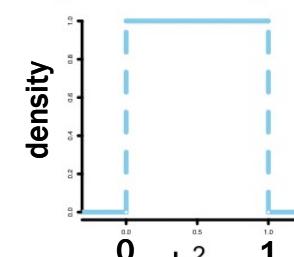
Simulations

Compare to observed data

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

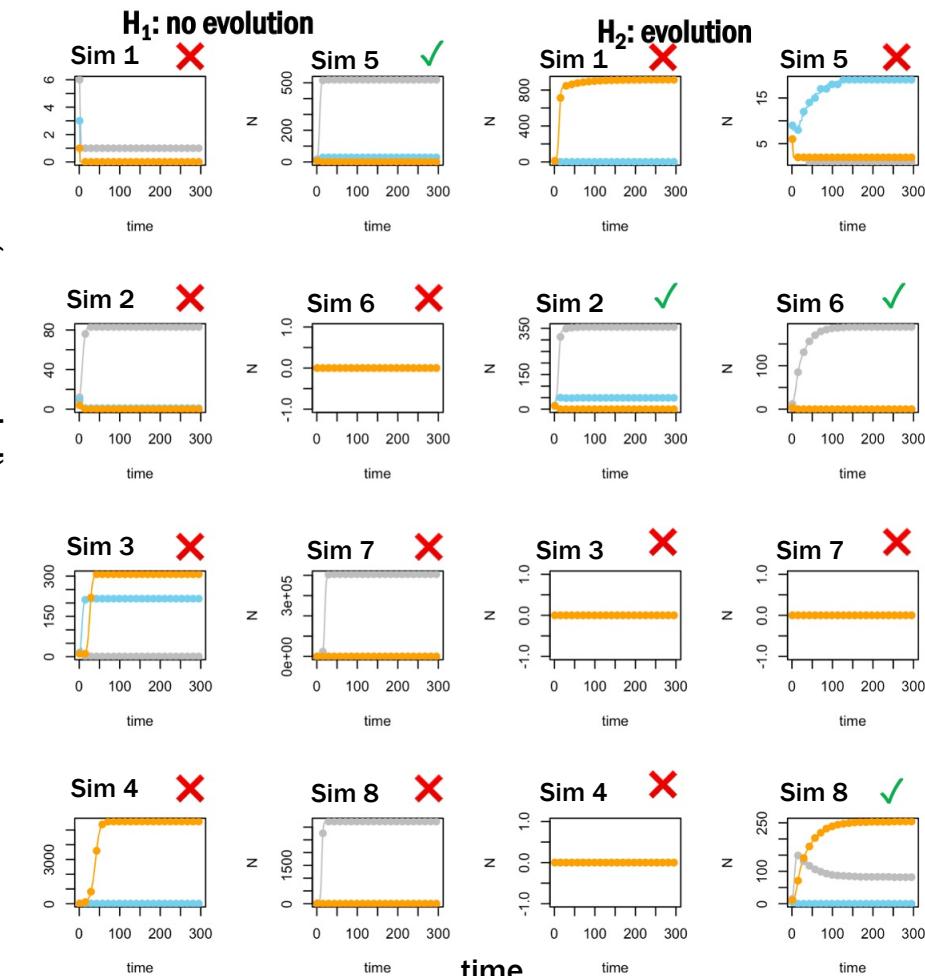
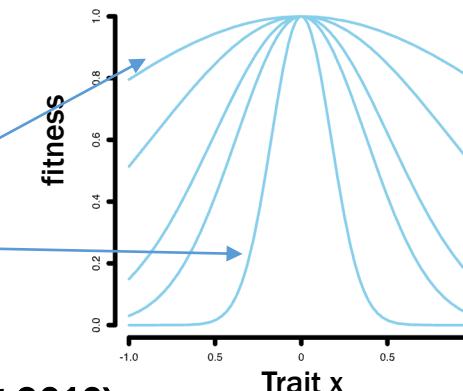
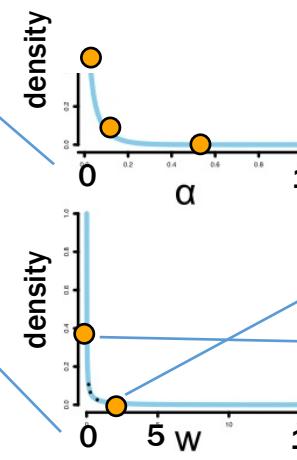


H_2 : Evolution ($h^2>0$)



interaction strength

strength of selection

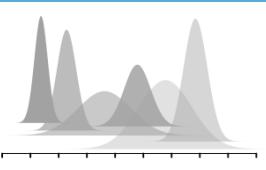


sample a candidate parameter vector θ^* from a proposed prior distribution, 100,000 simulations per model

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

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

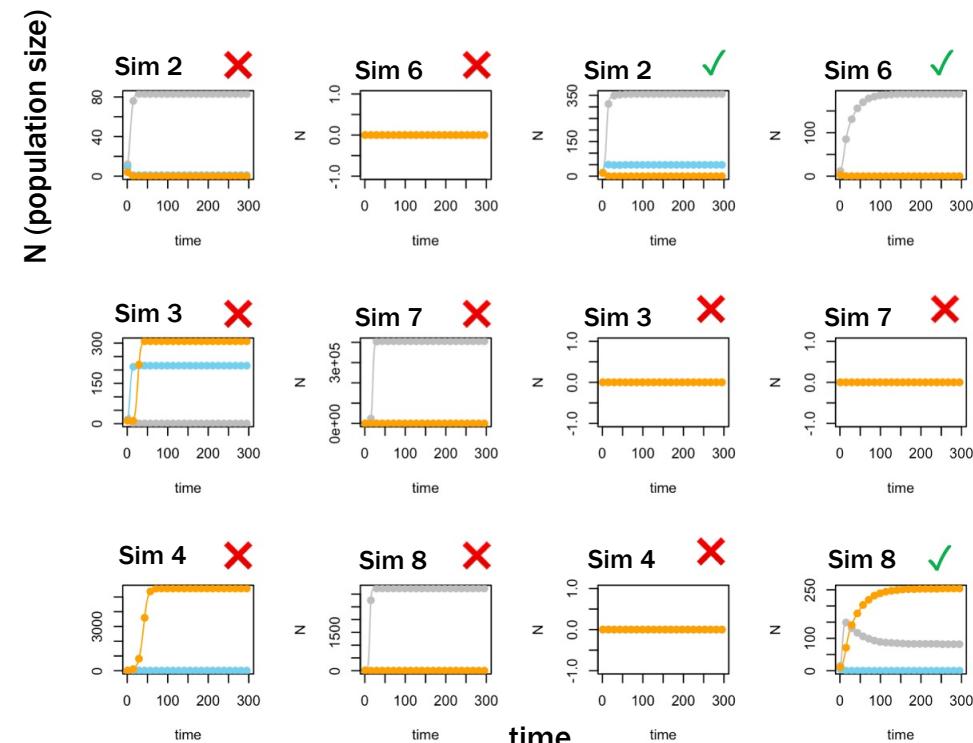
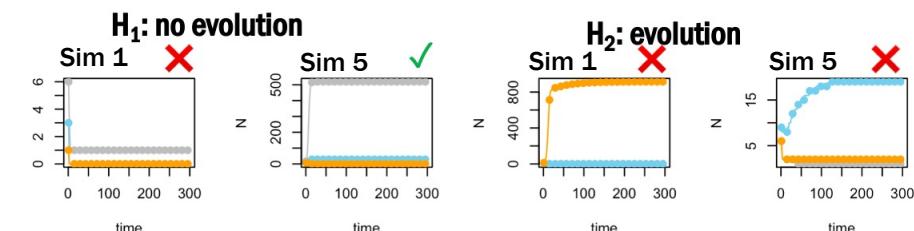
(i) Estimate posterior probability of alternative model hypotheses

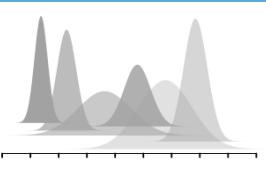
H_{eco}

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

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

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





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



Compare to observed data

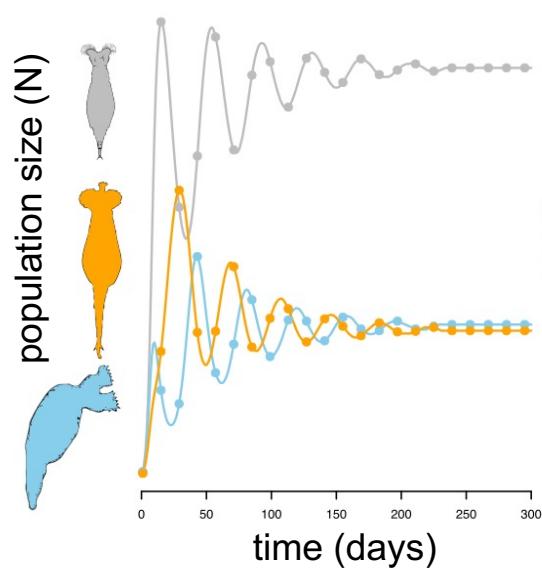
4. Compare observed data to alternative hypothesis simulations

(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

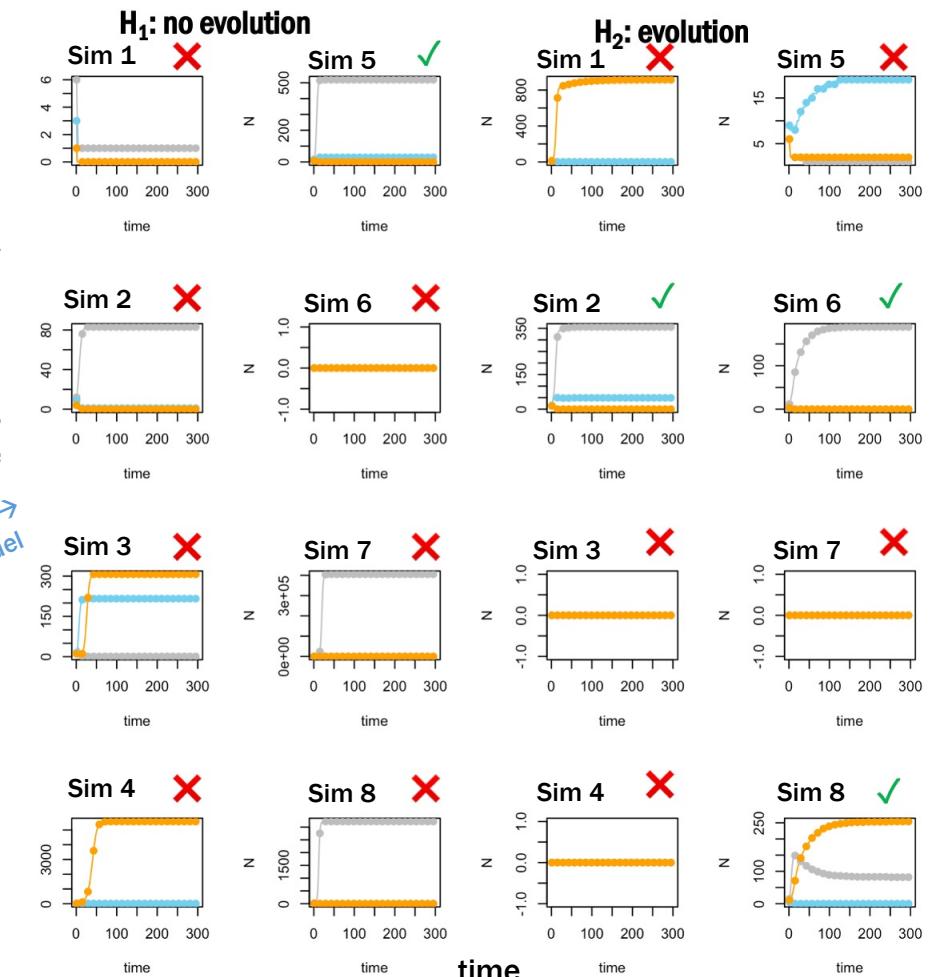
With x_0 and x_{300} trait values

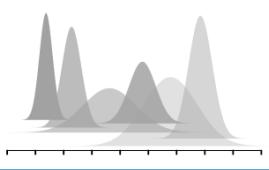


Posterior model probabilities for Observed Data

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

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

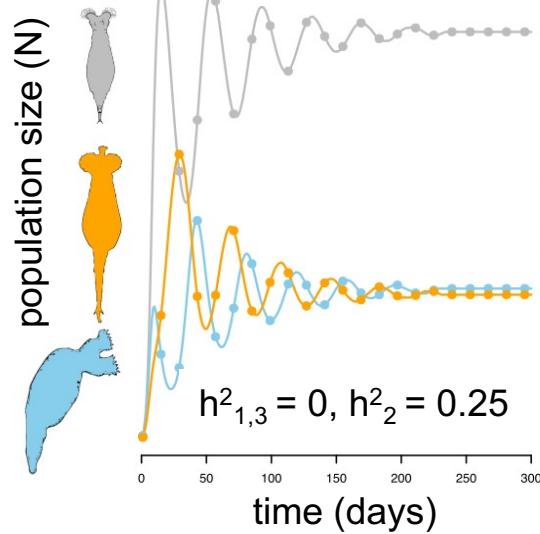
(i) Estimate posterior probability of alternative model hypotheses

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

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

Case 1. With simulated model + data

With x_0 and x_{300} trait values



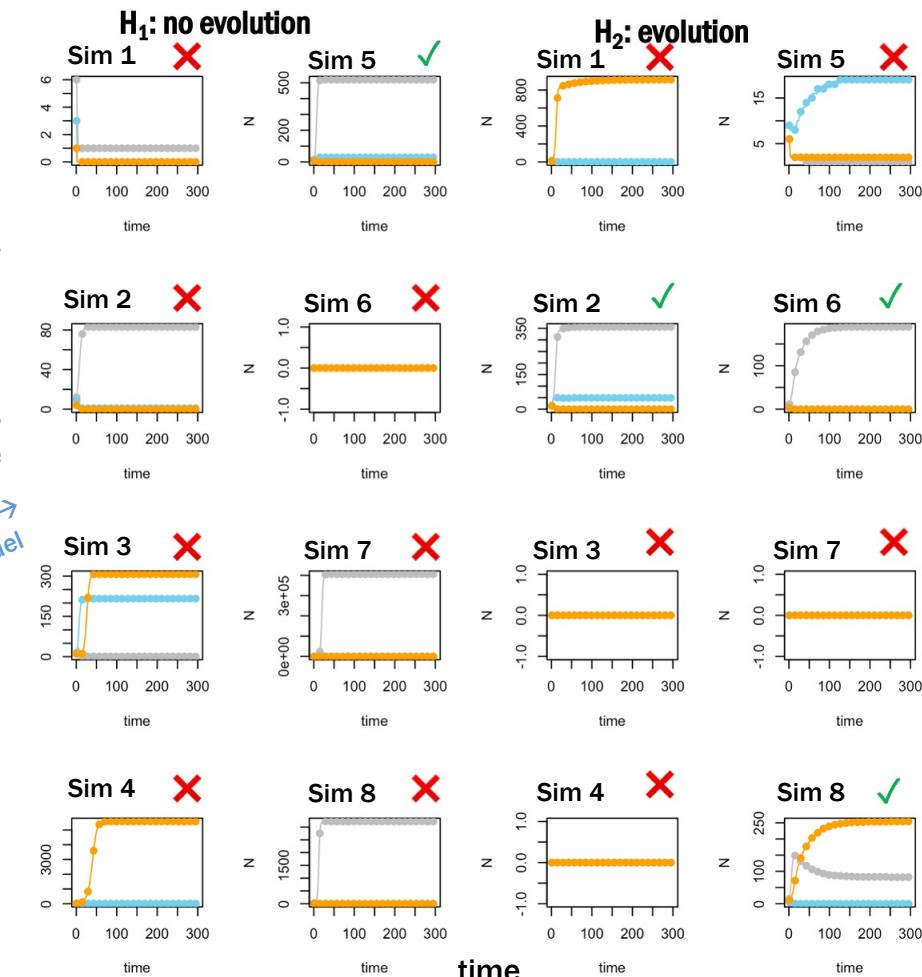
Posterior model probabilities for Observed Data

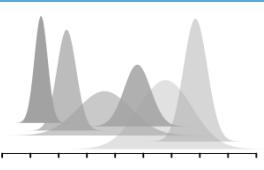
$$H_{\text{eco}} = 0.0001 \quad \times$$
$$H_{\text{eco-evo}} = 0.9999 \quad \checkmark$$

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

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

$$H_{\text{eco-evo}} = \frac{-[(\frac{w+(1-h^2)P}{P+w})(E-x_t)]^2}{2(P+w)} N_{i,t}$$

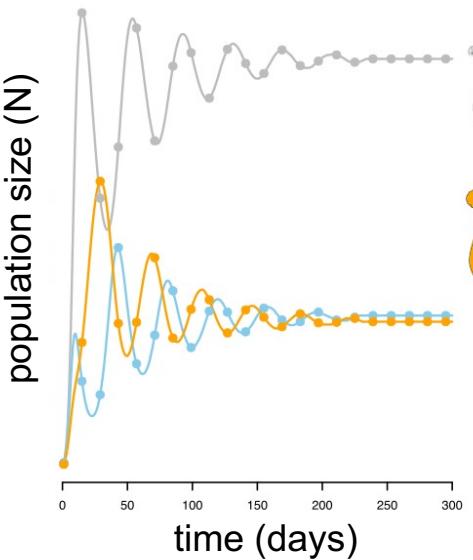
Case 2. With simulated model + data

With x_{300} trait values only (!!)

Posterior model probabilities for Observed Data

$$H_{\text{eco}} = 0.4676$$

$$H_{\text{eco-evo}} = 0.5324$$



Based on % Accepted vs. Rejected per H_A model

Case 3. With simulated model + data

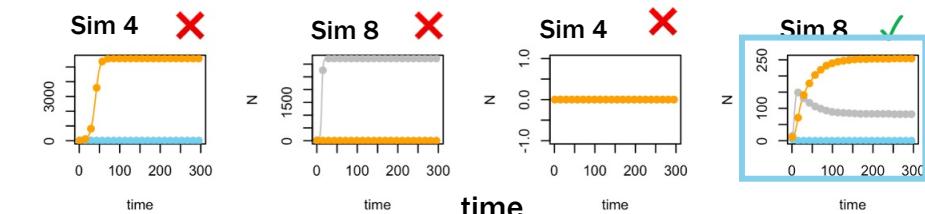
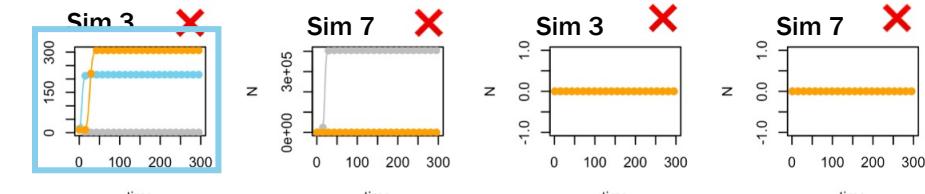
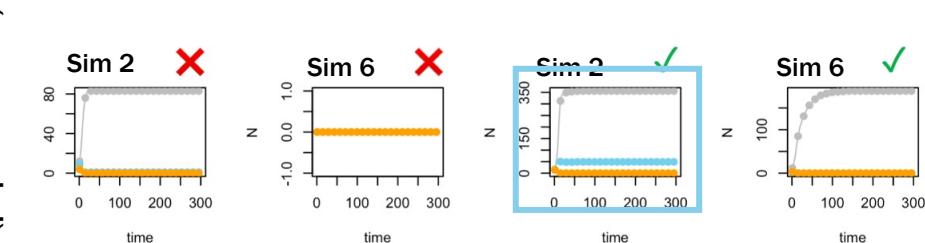
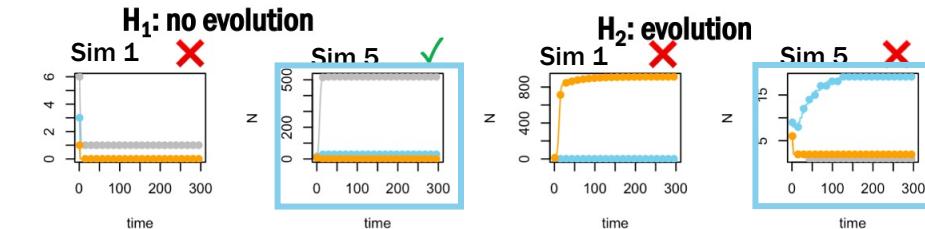
With x_{300} trait values only (!!)

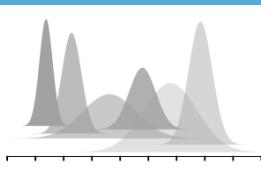
Restricted to 3-species persisting simulations only

Posterior model probabilities for Observed Data

$$H_{\text{eco}} = 0.0783$$

$$H_{\text{eco-evo}} = 0.9217$$





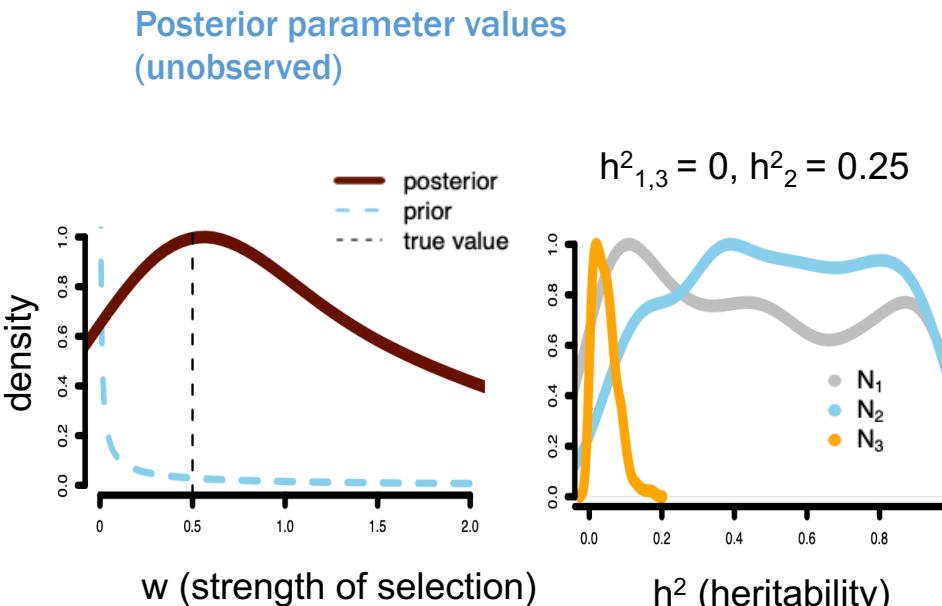
Research approach – eco-evolutionary hypothesis testing to fit data to models



Compare to observed data

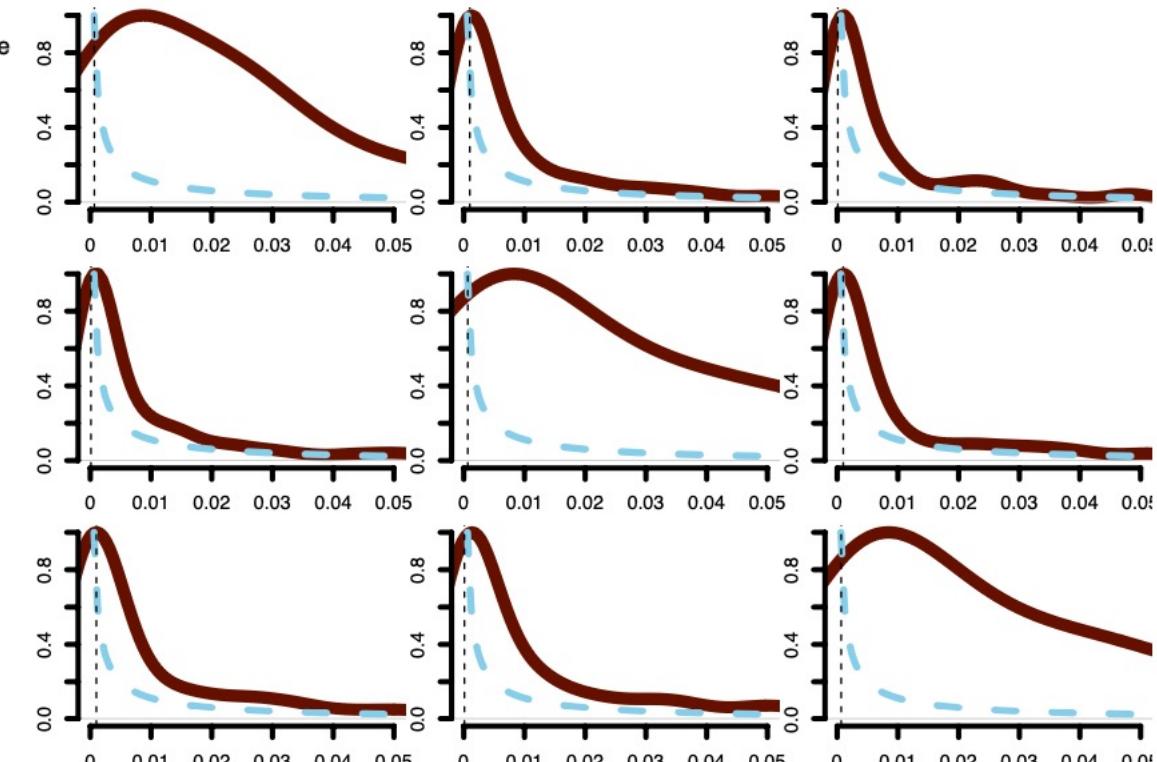
4. Compare observed data to alternative hypothesis simulations

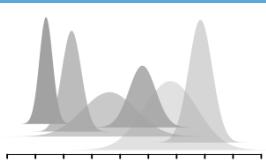
- (i) Estimate posterior probability of alternative model hypotheses
- (ii) Use best-fit (or consensus) models to estimate parameters for observed data, make predictions for future cases



posterior
prior
true value

$$\begin{bmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} = \begin{bmatrix} 0.000666 & 0.001 & 0.000111 \\ 0.000111 & 0.000666 & 0.001 \\ 0.001 & 0.000111 & 0.000666 \end{bmatrix}$$





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

