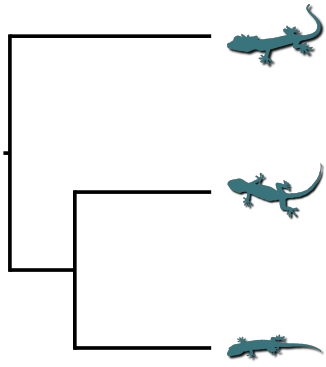
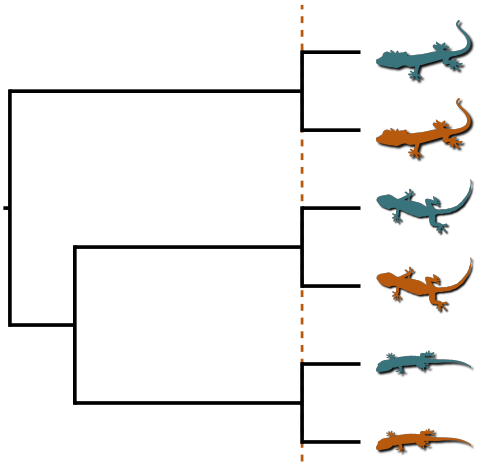
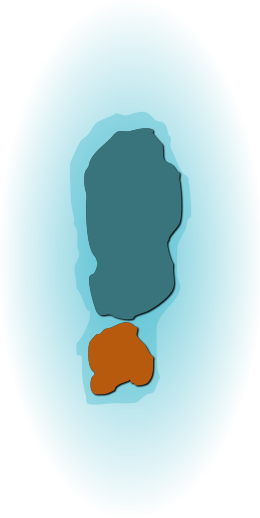
Exploring trait-dependent models of multi-lineage processes of diversification with machine learning

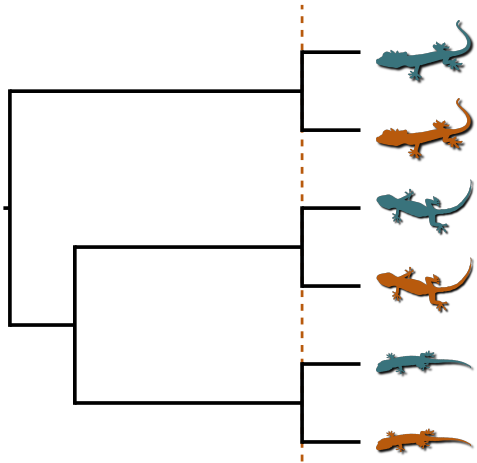
Jamie Oaks
Auburn University
phyletica.org
joaks1 & phyletica
@jamieoaks.bsky.social

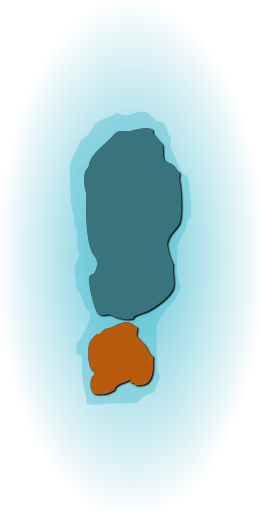
phyletica.org/slides/evol2025.pdf











*These "**shared**" or "**burst**" divergences violate assumption of independent divergences*

Biogeography

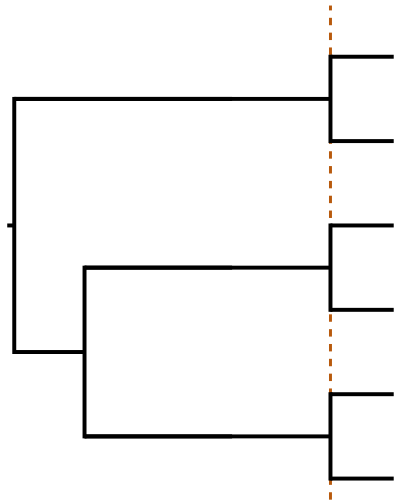
- Environmental changes that affect whole communities of species

Epidemiology

- Transmission at social gatherings

Genome evolution

- Duplication of a chromosome segment harboring a gene family



Biogeography

- Environmental changes that affect whole communities of species

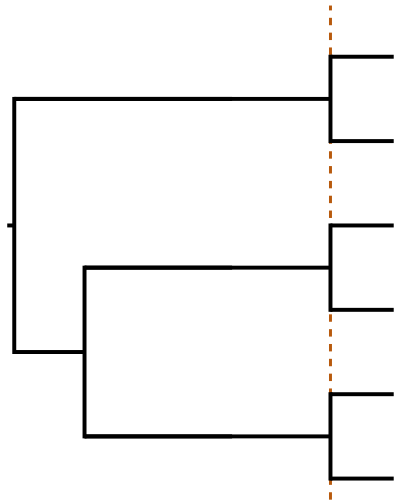
Epidemiology

- Transmission at social gatherings

Genome evolution

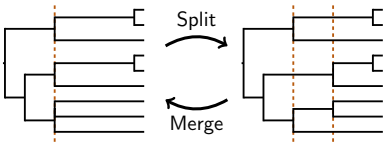
- Duplication of a chromosome segment harboring a gene family

These processes are interesting!

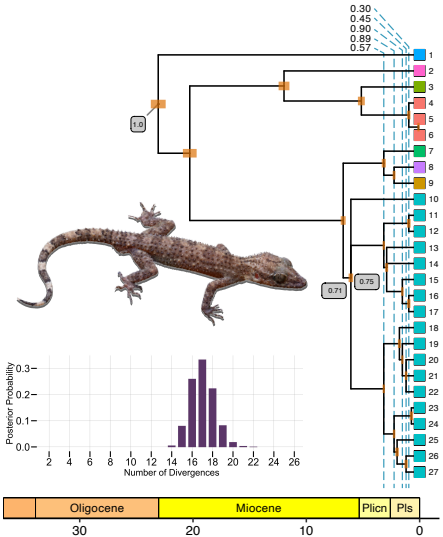


Progress on shared divergences: Phycoeval

Phycoeval



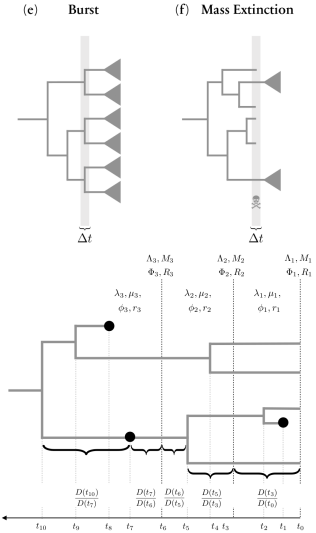
- Bayesian inference of trees with shared divergences



J. R. Oaks et al. (2022). *PNAS* 119: e2121036119

Progress on shared divergences: Birth-Death + Bursts

- Andrew Magee & Sebastian Höhna
- Likelihood of tree under BD model with "burst" events



A. F. Magee et al. (2021). *bioRxiv*

Motivating questions

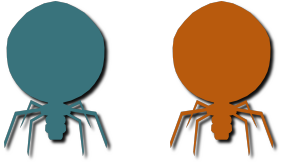
- Did geckos adapted to karst diversify via fragmentation of karst formations?

Credit: Perry Wood, Jr.; phylopic.org CC0

Motivating questions

- Did geckos adapted to karst diversify via fragmentation of karst formations?

- Do viral strains differ in ability to spread at social gatherings?

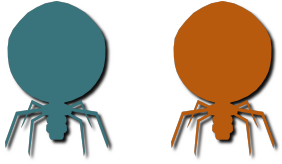


Credit: Perry Wood, Jr.; phylopic.org CC0

Motivating questions

- Did geckos adapted to karst diversify via fragmentation of karst formations?

- Do viral strains differ in ability to spread at social gatherings?

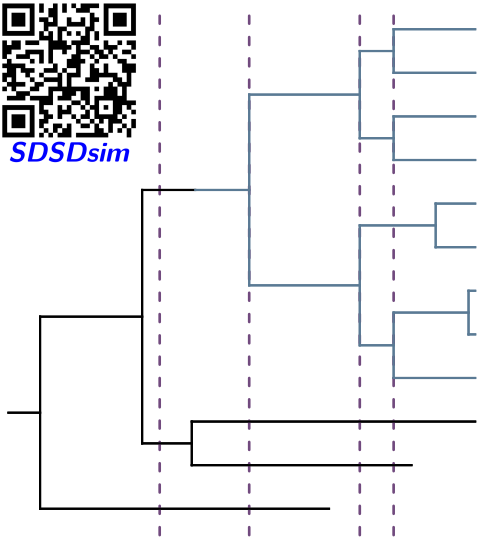


These questions require state-dependent models

Credit: Perry Wood, Jr.; phylopic.org CC0

State-dependent model of shared divergences

SDSDsim

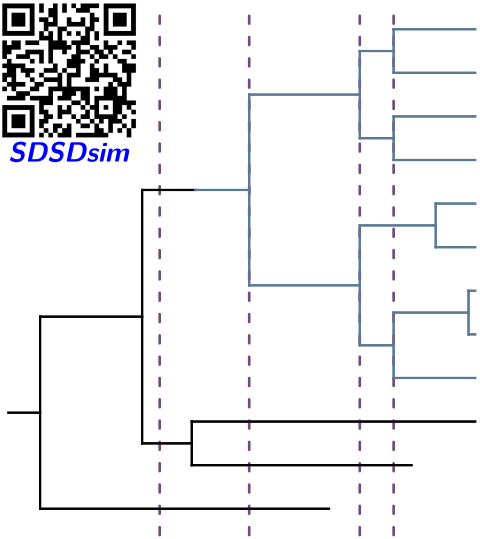


Parameters:

- Transition rates between character **State 0** ⇆ **State 1**
- Speciation rate, λ (per-lineage)
- Extinction rate, μ (per-lineage)
- Rate of "burst events", β (tree-wide)
- **State 0** probability of speciation at events, p_0
- **State 1** probability of speciation at events, p_1

State-dependent model of shared divergences

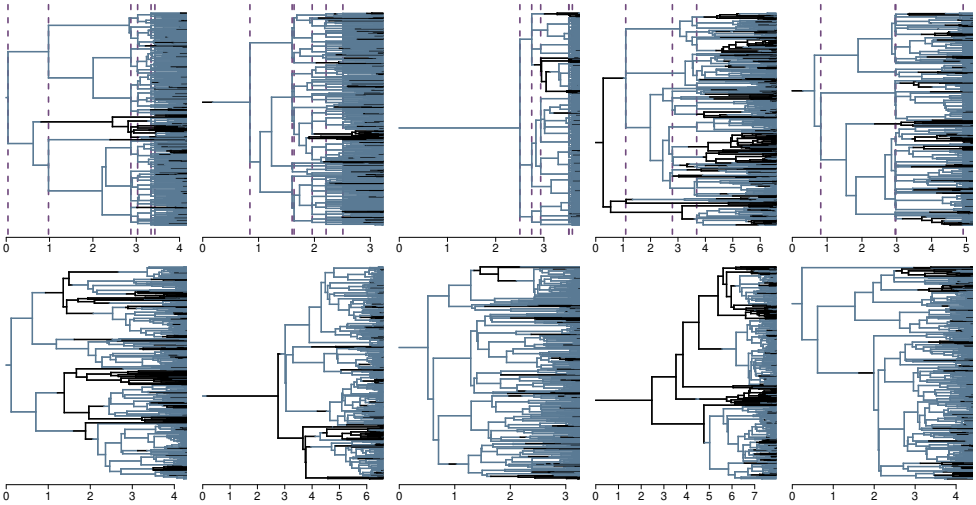
SDSDsim



Parameters:

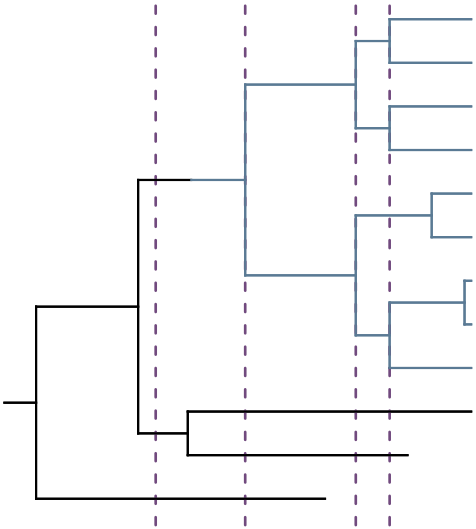
- Transition rates between character **State 0** ⇆ **State 1**
- Speciation rate, λ (per-lineage)
- Extinction rate, μ (per-lineage)
- Rate of "burst events", β (tree-wide)
- **State 0** probability of speciation at events, p_0
- **State 1** probability of speciation at events, p_1
  - $p_1\beta$ = Per-lineage expected rate of burst divergences

Some random example trees



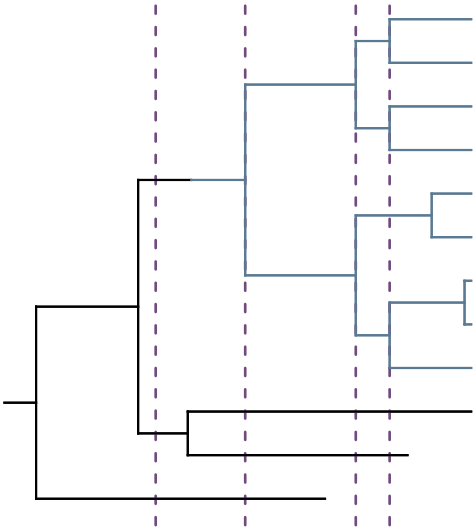
Both models have same expected rates of state-dependent diversification

What next?



Ideally, full Bayesian inference of state-dependent burst model and tree

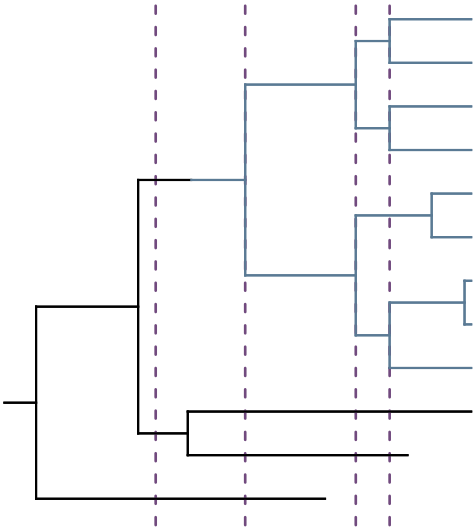
What next?



Ideally, full Bayesian inference of state-dependent burst model and tree

That's a lot of work...

What next?



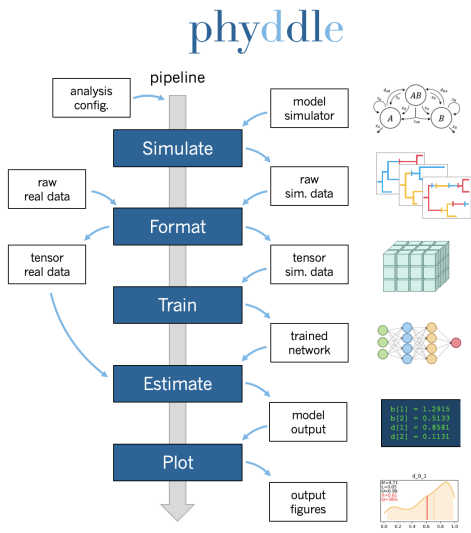
Ideally, full Bayesian inference of state-dependent burst model and tree

That's a lot of work...

Is it worth it?

- Is there information in the trees to detect shared divergence rates and state-dependent differences?

- User-friendly deep learning with trees
- Ammon Thompson & Michael Landis



A. Thompson et al. (2024). *Systematic Biology* 73: 183–206, M. J. Landis et al. (2025). *Systematic Biology*. syaf036

phyddle analyses

- Simulated 100k, trees (95k training, 5k holdout) with 500 extant tips
  - Extinct lineages removed
- Speciation rate, $\lambda \sim$ Log-uniform$(0.01, 1)$
- Extinction rate $\sim$ Log-uniform$(0.01\lambda, \lambda)$
- Two character states
  - Transition rate $\sim$ Uniform$(0.1\lambda, 0.7\lambda)$

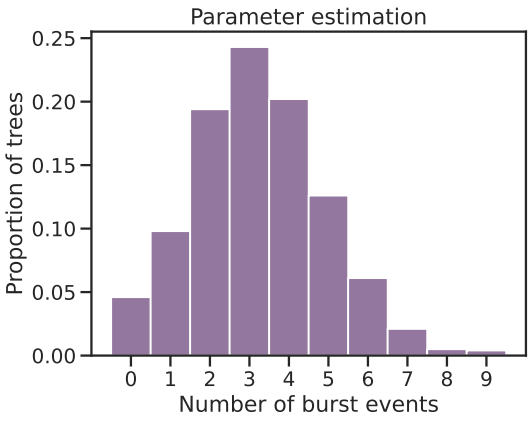
Parameter estimation

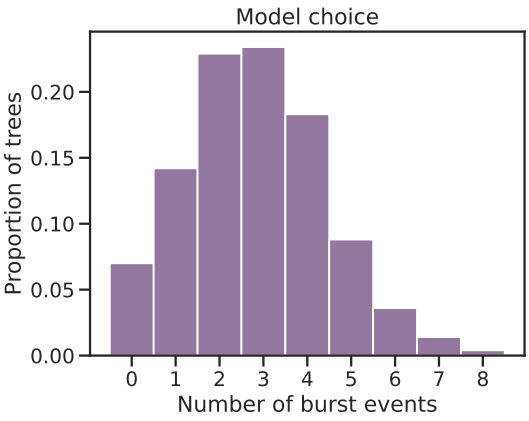
- Burst rate $\sim$ Uniform$(0.3\lambda, 1.2\lambda)$
- State 0 burst prob $\sim$ Uniform$(0.65, 1)$
- State 1 burst prob $\sim$ Uniform$(0.1, 0.65)$

Model choice

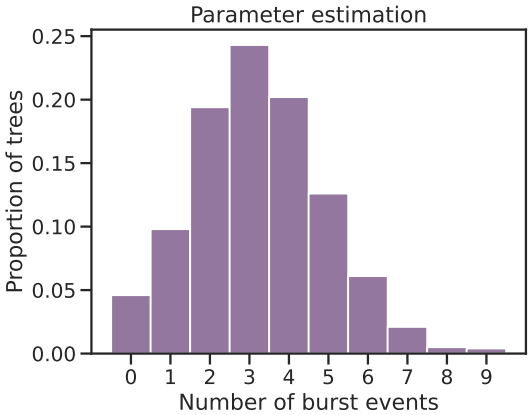
- Burst rate $\sim$ Uniform$(0.2\lambda, \lambda)$
- State 0 burst prob $\sim$ Uniform$(0.6, 1)$
- State 1 burst prob $=$ State 0
  OR $\sim$ Uniform$(0.0, 0.3)$

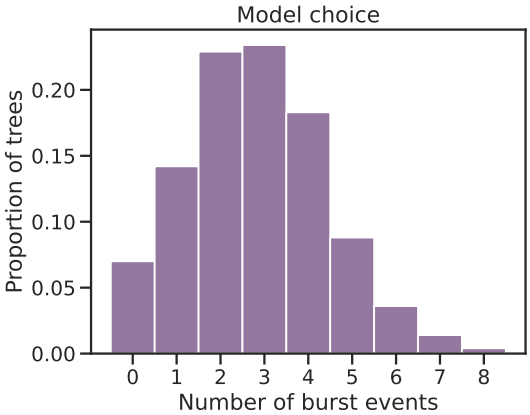
Results: Number of burst events





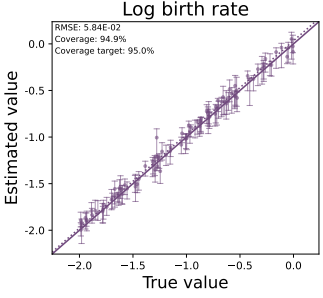
Results: Number of burst events

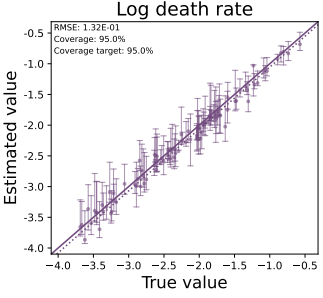


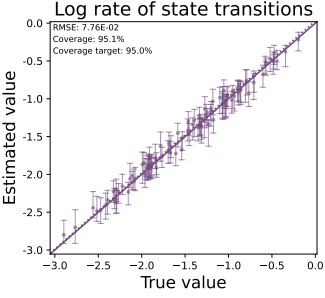


The simulated trees do not have large numbers of burst events to learn from

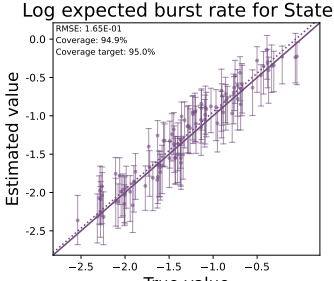
Results: State-dependent burst ***parameter estimation***

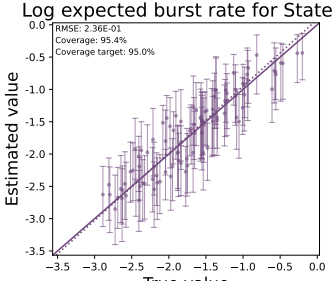


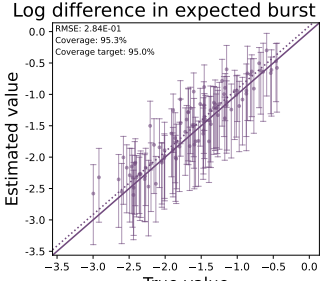


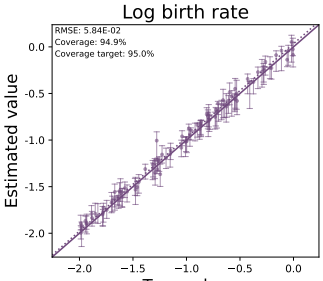


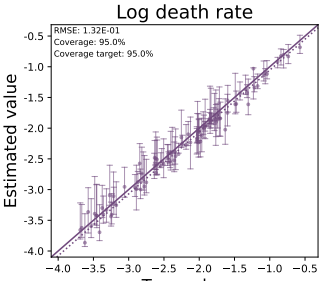
Results: State-dependent burst ***parameter estimation***

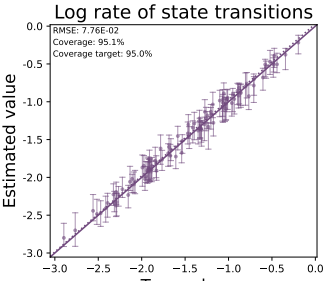




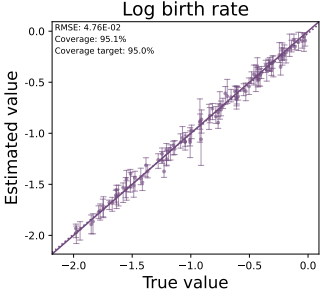


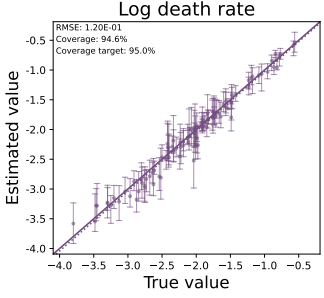


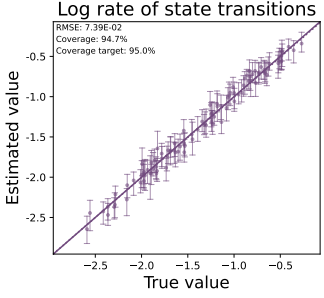




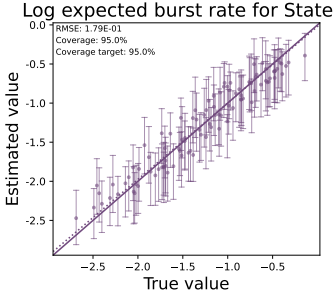
Results: State-dependent burst ***model choice***

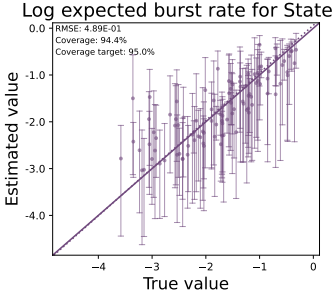


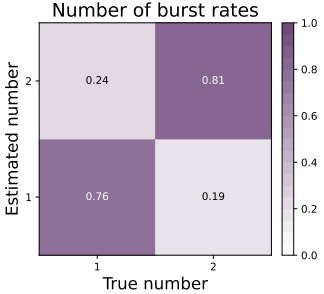


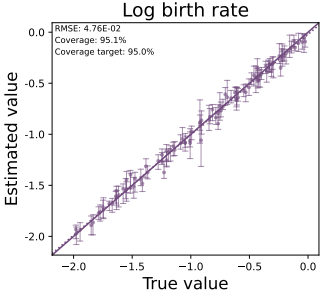


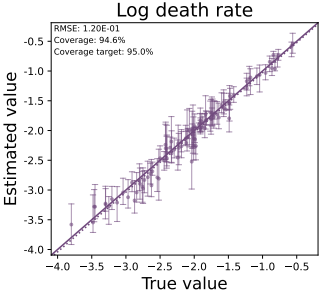
Results: State-dependent burst ***model choice***

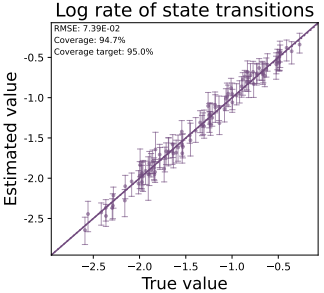




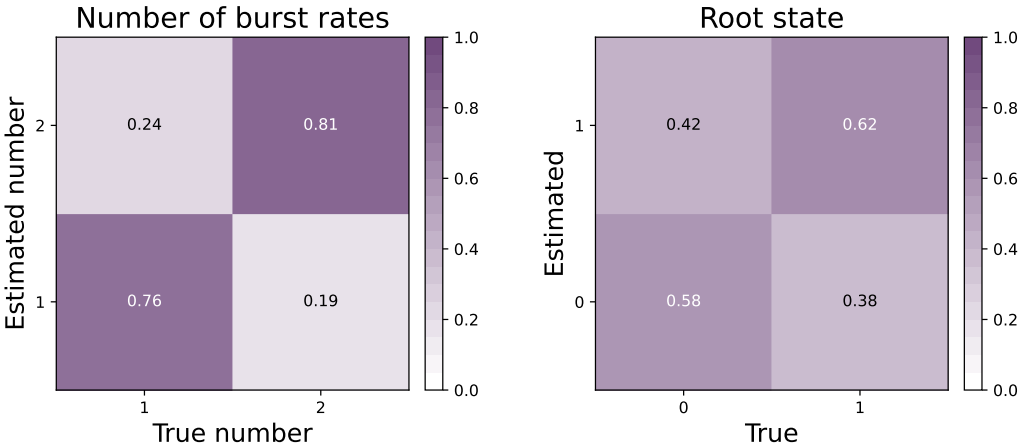








Results: State-dependent burst ***model choice***



Estimating burst model better than ancestral state**

Take-homes

Trees generated by a BD model with state-dependent burst rates have information about those burst rates

phyddle is a user-friendly tool for quickly experimenting with new (hair-brained) phylogenetic models

Caveats:

- Analyses assumed no model violations
- Trees aren't observable!

Next steps

Introduce polytomies into burst events

- Burst-y processes predict them
  - *E.g.*, Do rising sea levels always split one island into two?
  - *E.g.*, Does a carrier always infect one other individual at a social gathering?

Next steps

Introduce polytomies into burst events

- Burst-y processes predict them
  - *E.g.*, Do rising sea levels always split one island into two?
  - *E.g.*, Does a carrier always infect one other individual at a social gathering?

Develop full Bayesian implementation of state-dependent shared divergence models

- Learn from actual data (sequences) while integrating phylo uncertainty
- Can make probability statements about events within the tree
  - The neural network is trained on random trees

Open science: everything is available. . .

Simulator:

github.com/phyletica/SDSDsim

Open-science notebook:

github.com/phyletica/SDSDsim-phyddle-experiments

Shout-outs

- Phyletica Lab (the Phyleticians)
- Perry Wood, Jr.
- Ammon Thompson
- Michael Landis
- Sebastian Höhna

Computation:

- Alabama Supercomputer Authority
- Auburn University Easley Cluster

Photo credits:

- Perry Wood, Jr.
- PhyloPic

Questions?

joaks@auburn.edu

Slides:

phyletica.org/slides/evol2025.pdf