Phylogenetic model comparison (by) selection & averaging

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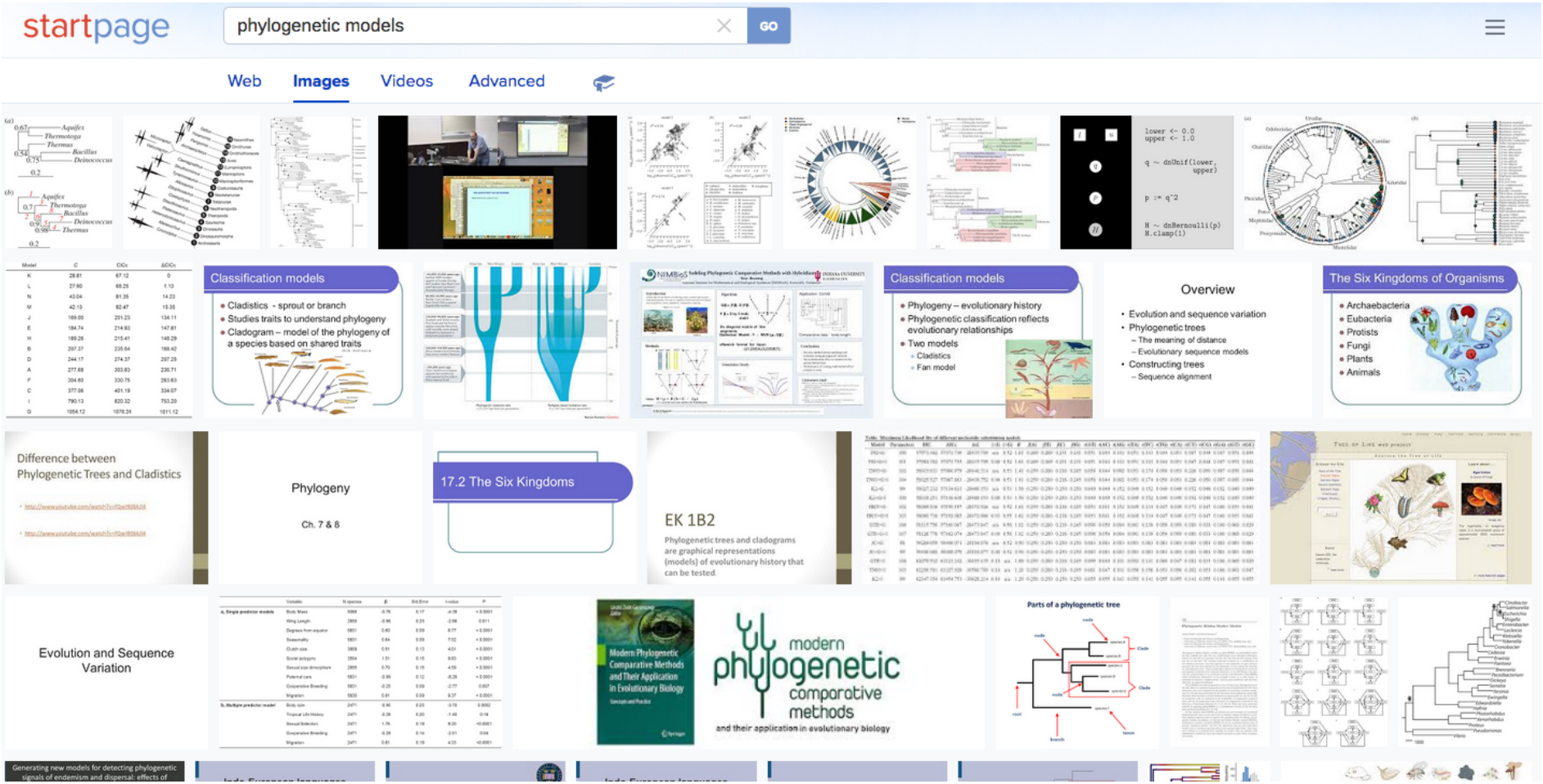
- Model averaging
- Model selection
- Model comparison

What does a model look like

Model = tree prior + site model + clock model + *priors* + *hyper priors*



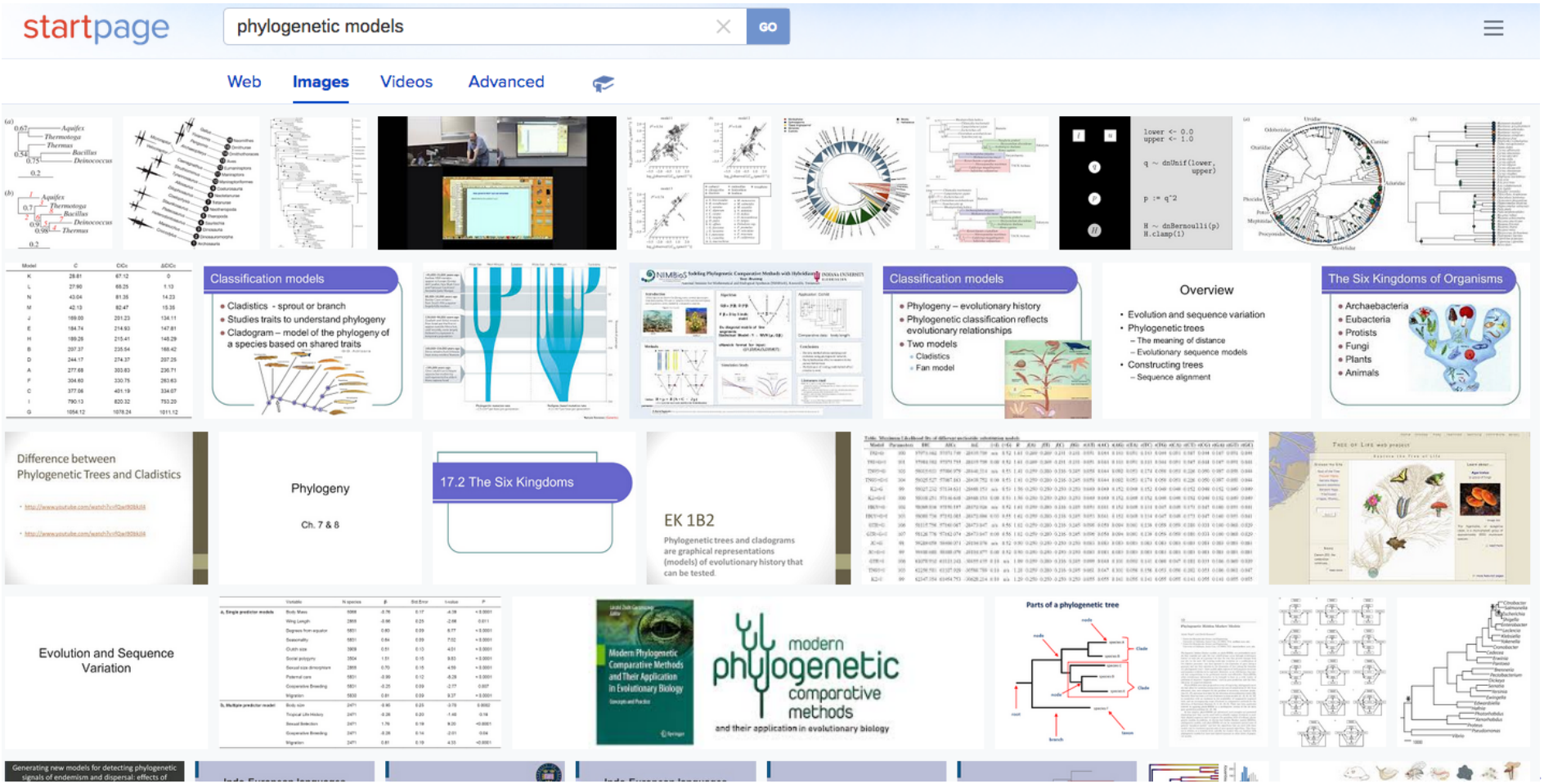
What does a model look like

Model Comparison: Which one is better?

Model Selection: Which one to pick?

Model Averaging: What if you don't want to choose?

Model = tree prior + site model + clock model + *priors* + *hyper priors*



Model averaging

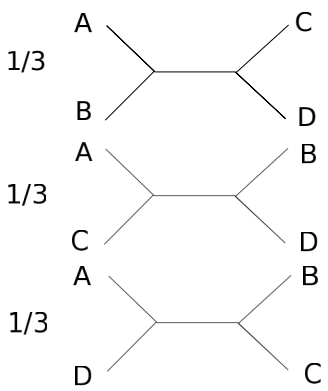
- Posterior:

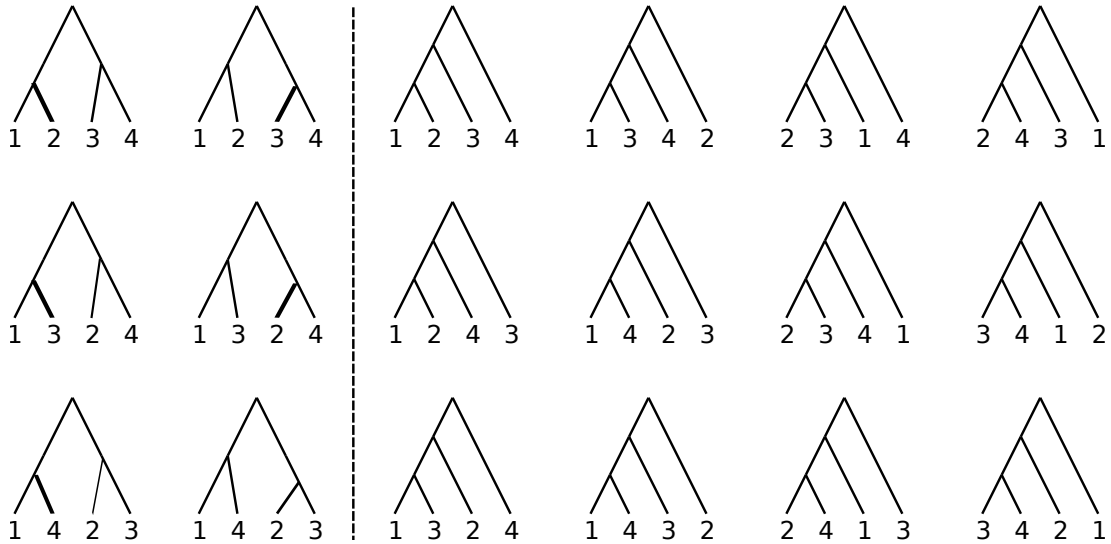
$$p(\theta|D) = \sum_k \overbrace{P(M_k)}^{\text{model prior}} \underbrace{\pi(\theta|M_k)L(D|M_k,\theta)}_{\text{posterior}}$$

- Models can be substitution models, clock models, tree topologies, etc.
- Accounts for model uncertainty
- Requires specifying another prior $P(M_k)$

Model averaging

Already been doing that this all week: each tree topology is a model





18 ranked rooted trees – 1/3 probability of being balanced

Model averaging: stochastic variable selection

Use indicator variable to select model

- Example: ancestral state reconstruction using mask matrix I and rate matrix R

$$I = \begin{pmatrix} - & i_{12} & i_{13} & i_{14} \\ i_{21} & - & i_{23} & i_{24} \\ i_{31} & i_{32} & - & i_{34} \\ i_{41} & i_{42} & i_{43} & - \end{pmatrix} \qquad R = \begin{pmatrix} - & r_{12} & r_{13} & r_{14} \\ r_{21} & - & r_{23} & r_{24} \\ r_{31} & r_{32} & - & r_{34} \\ r_{41} & r_{42} & r_{43} & - \end{pmatrix}$$

- Use r_{ij} is i_{ij} is true, but use rate 0 if i_{ij} is false
- Sample I and all rates in R throughout MCMC run.
- Use strong prior on number of $i_{ij} = true$ to reduce number of non-zero rates

Lemey et al, PLoS Comput Biol, 2009

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Stochastic variable selection:

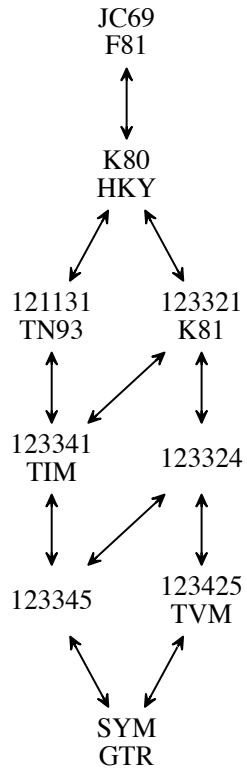
- Simple to implement
- Potentially inefficient in sampling unused parameters

Model averaging: reversible jump

The probability of acceptance of a (possibly trans-dimensional) proposal is

$$\min\{1, \text{posterior ratio} \times \text{proposal ratio} \times \text{Jacobian}\}$$

- **posterior ratio** is the posterior of the proposed state S' divided by that of the current state S,
- **proposal ratio** the probability of moving from S to S' divided by the probability of moving back from S' to S
- **Jacobian** is the determinant of the matrix of partial derivatives of the parameters in the proposed state with respect to that of the current state Green, Biometrika, 1995



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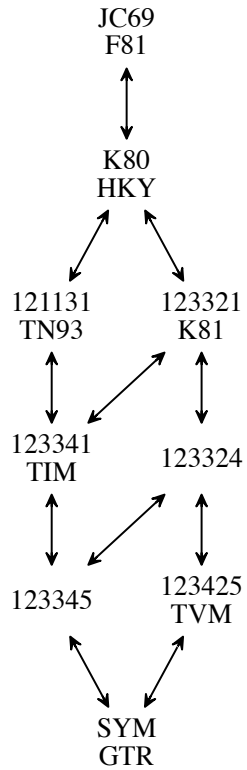


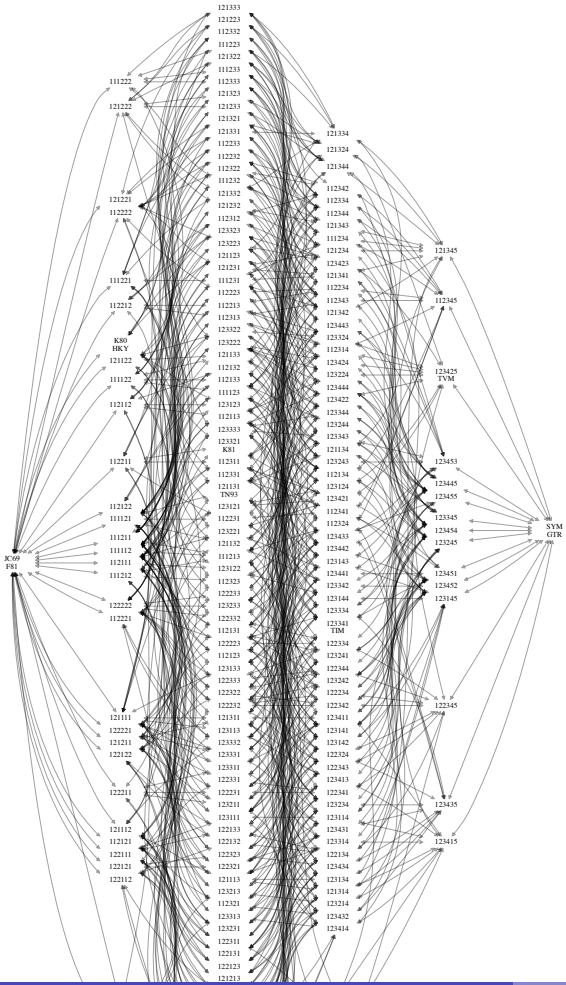
Reversible jump:

- Hard to implement correctly
- Efficient sampling

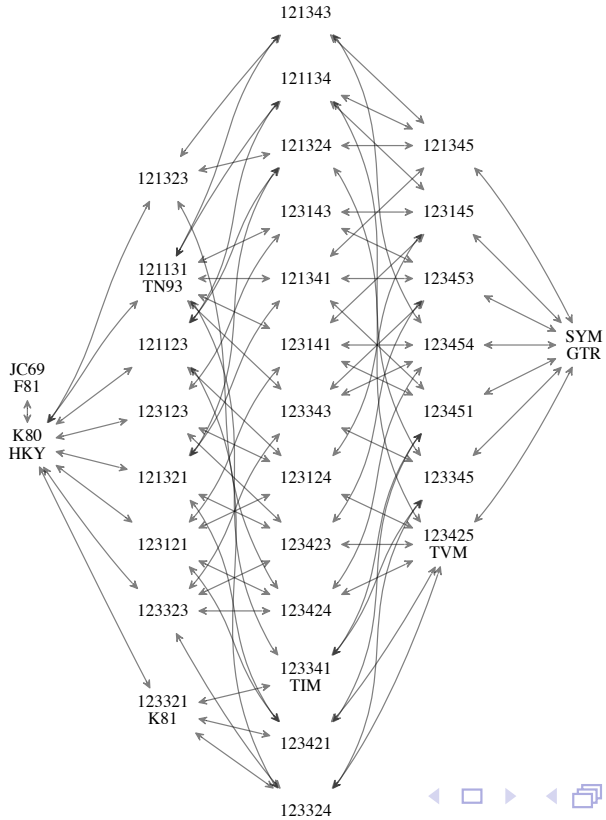
Model averaging: bModelTest Bouckaert & Drummond, BMC Evo Bio, 6 Feb 2017

- Averages over substitution models
- Estimated/fixed frequencies
- With/without gamma rate heterogeneity
- With/without gamma proportion invariable sites

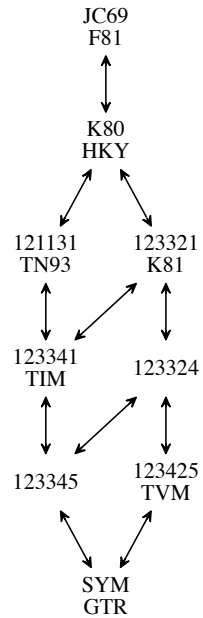
(a)



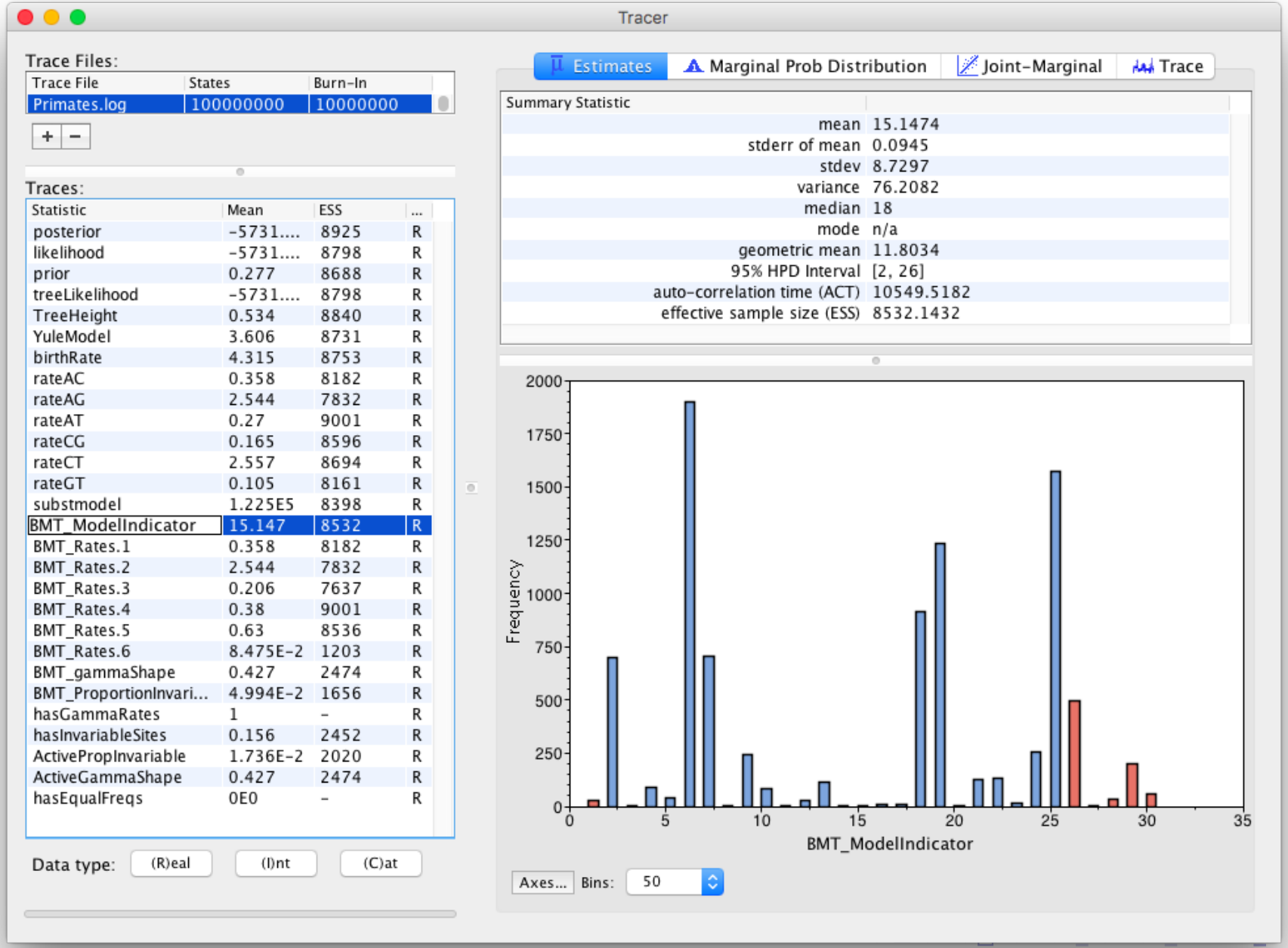
(b)



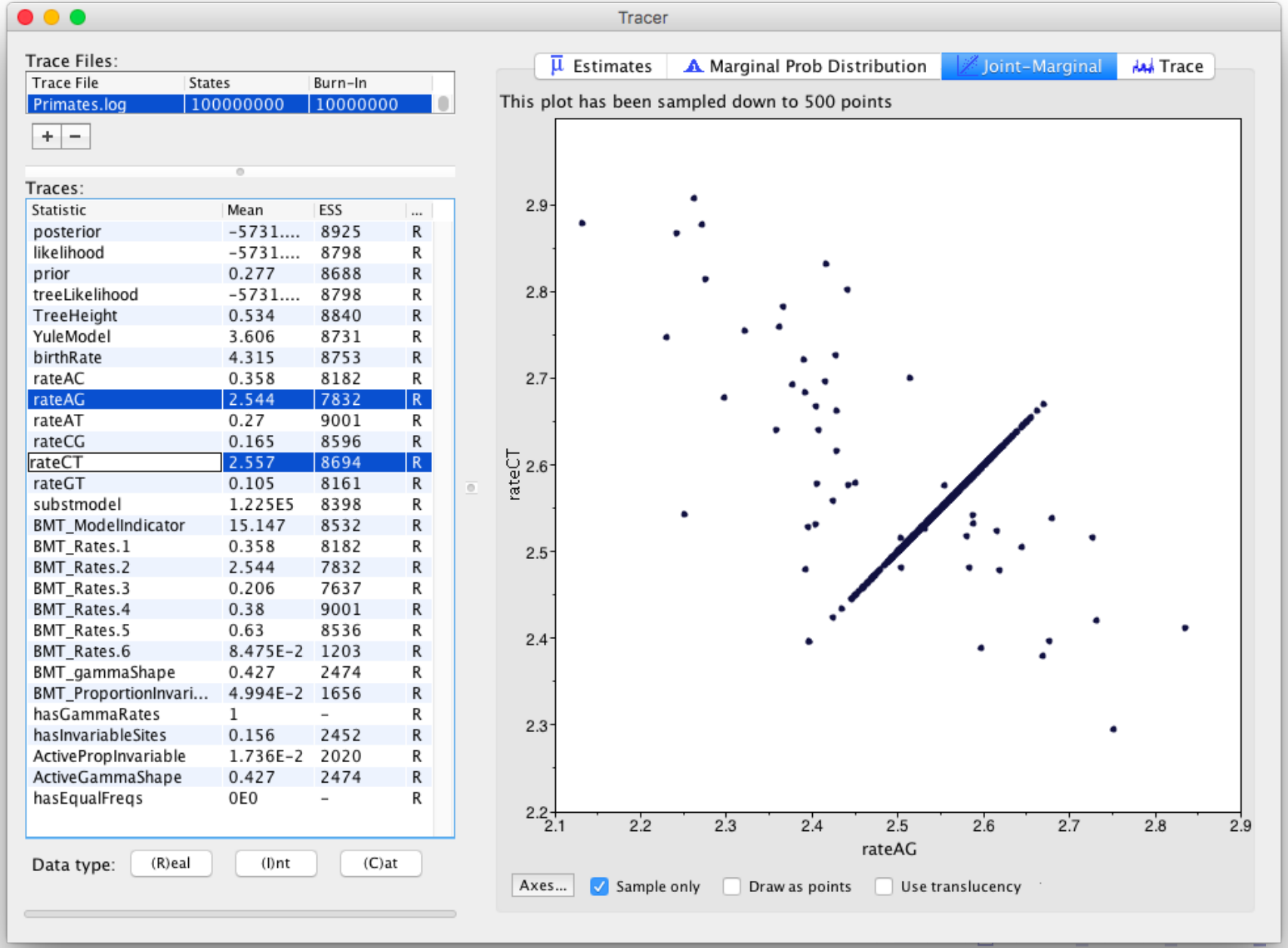
(c)



Model averaging: bModelTest



Model averaging: bModelTest

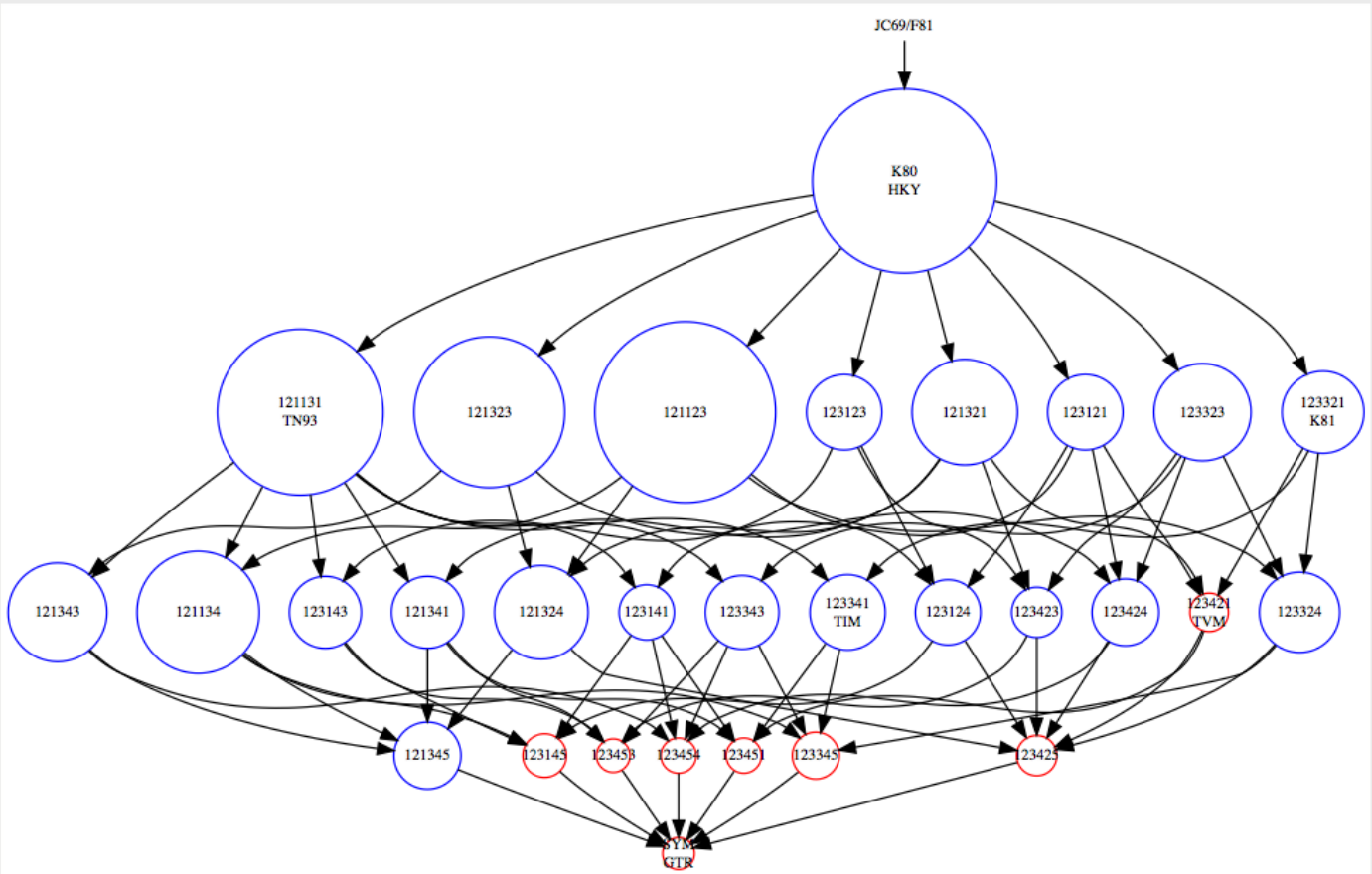


Model averaging: bModelTest

File: Primates.log item: substmodel

Models with blue circles are inside 95%HPD, red outside, and without circles have 0.00% support.

posterior support	cumulative support	model
13.77%	13.77%	121121
13.21%	26.99%	121123
11.16%	38.15%	121131
9.27%	47.42%	121323
6.05%	53.47%	121134
4.44%	57.91%	121321
3.94%	61.85%	121343
3.78%	65.63%	123323
3.50%	69.13%	121324
2.72%	71.85%	123321
2.61%	74.46%	123324
2.33%	76.79%	123121
2.28%	79.07%	123123
2.28%	81.34%	123341
2.17%	83.51%	123343
2.05%	85.56%	121341
2.05%	87.62%	123143
1.83%	89.45%	123424
1.78%	91.23%	121345
1.72%	92.95%	123124
1.22%	94.17%	123141
1.05%	95.22%	123423
0.89%	96.11%	123345

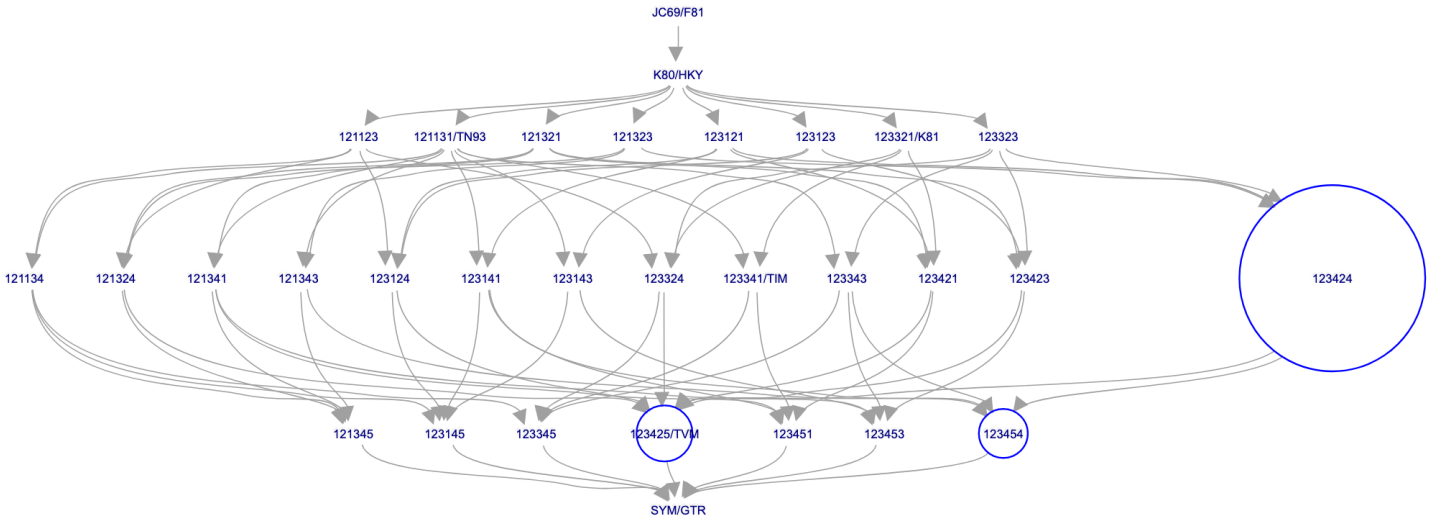


Model averaging: bModelTest

File: hbvz-bmt-cexp.log item: substmodel

Models with blue circles are inside 95%HPD, red outside, and without circles have at most 0.34% support.

posterior support	cumulative support	model
85.91%	85.91%	123424
7.79%	93.70%	123425
5.96%	99.66%	123454
0.34%	100.00%	123456



Model averaging: bModelTest model priors

Posterior:

$$p(\theta|D) = \sum_k P(M_k)\pi(\theta|M_k)L(D|M_k,\theta)$$

$P(M_k)$ model prior:

- uniform over substitution models in model set
  - For 31 model set: $P(JC) = P(HKY) = P(TN) = P(GTR) = \frac{1}{31}$
- uniform over number of parameters in substitution models
  - For 31 model set: $P(JC) = P(HKY) = P(GTR) = \frac{1}{6}$ but $P(TN) = \frac{1}{6}\frac{1}{8} = \frac{1}{48}$

Model selection

When to do model selection:

- answers of interest are not robust for different models
- to test hypotheses (encoded by prior)
- not because the reviewers demand it

Evade it if you can

Model selection

Measures of fit:

- Super naive: compare posteriors
  - priors are not normalised, so posteriors cannot be compared
  - Never do this!

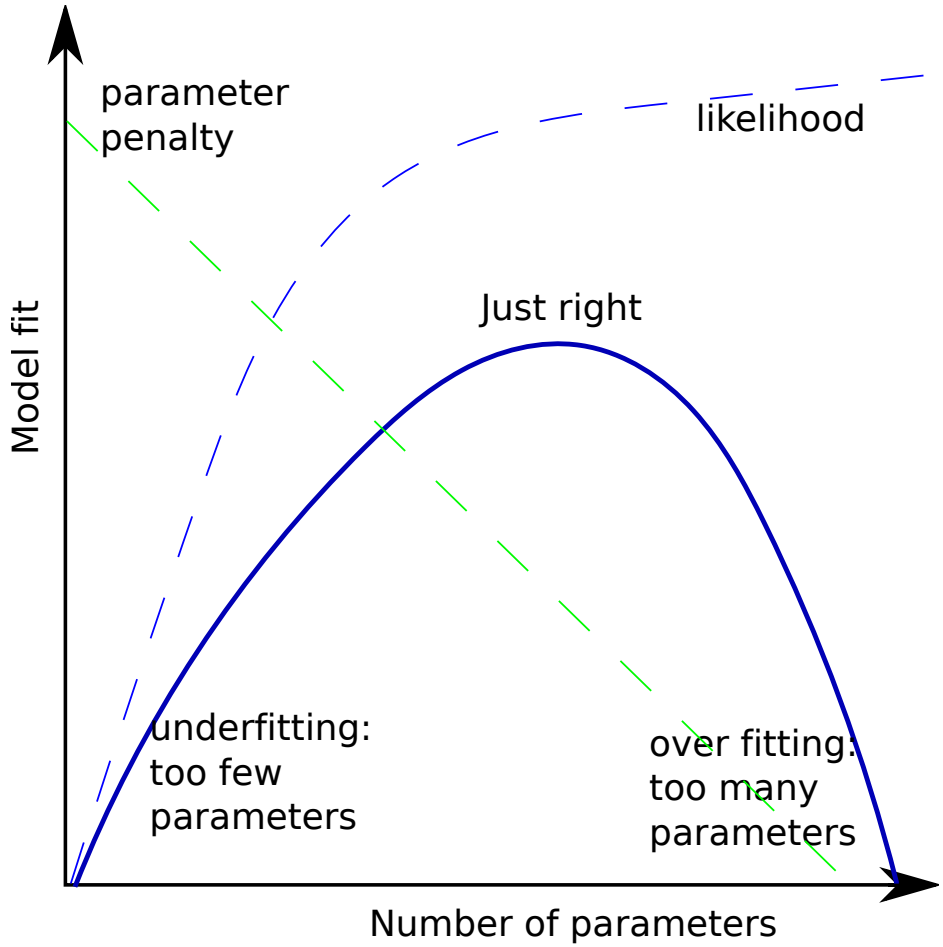
Model selection

Measures of fit:

- Super naive: compare posteriors
  - priors are not normalised, so posteriors cannot be compared
  - Never do this!
- Super naive: compare likelihoods
  - overparameterisation/overfitting cannot be detected
  - Never do this!

Model selection: select model with best "fit"

Desirable model fit property 1: likelihood - parameter penalty



Desirable model fit property 2: replicability/low variance

Desirable model fit property 3: easy & cheap to calculate

(this list is not exhaustive)

Bayesian model selection: marginal likelihood

Posterior:

$$p(\theta|D,M) = \frac{\overbrace{\pi(\theta|M)}^{\text{prior}}\overbrace{L(D|M,\theta)}^{\text{likelihood}}}{\underbrace{p(D|M)}_{\text{marginal likelihood}}}$$

Marginal likelihood:

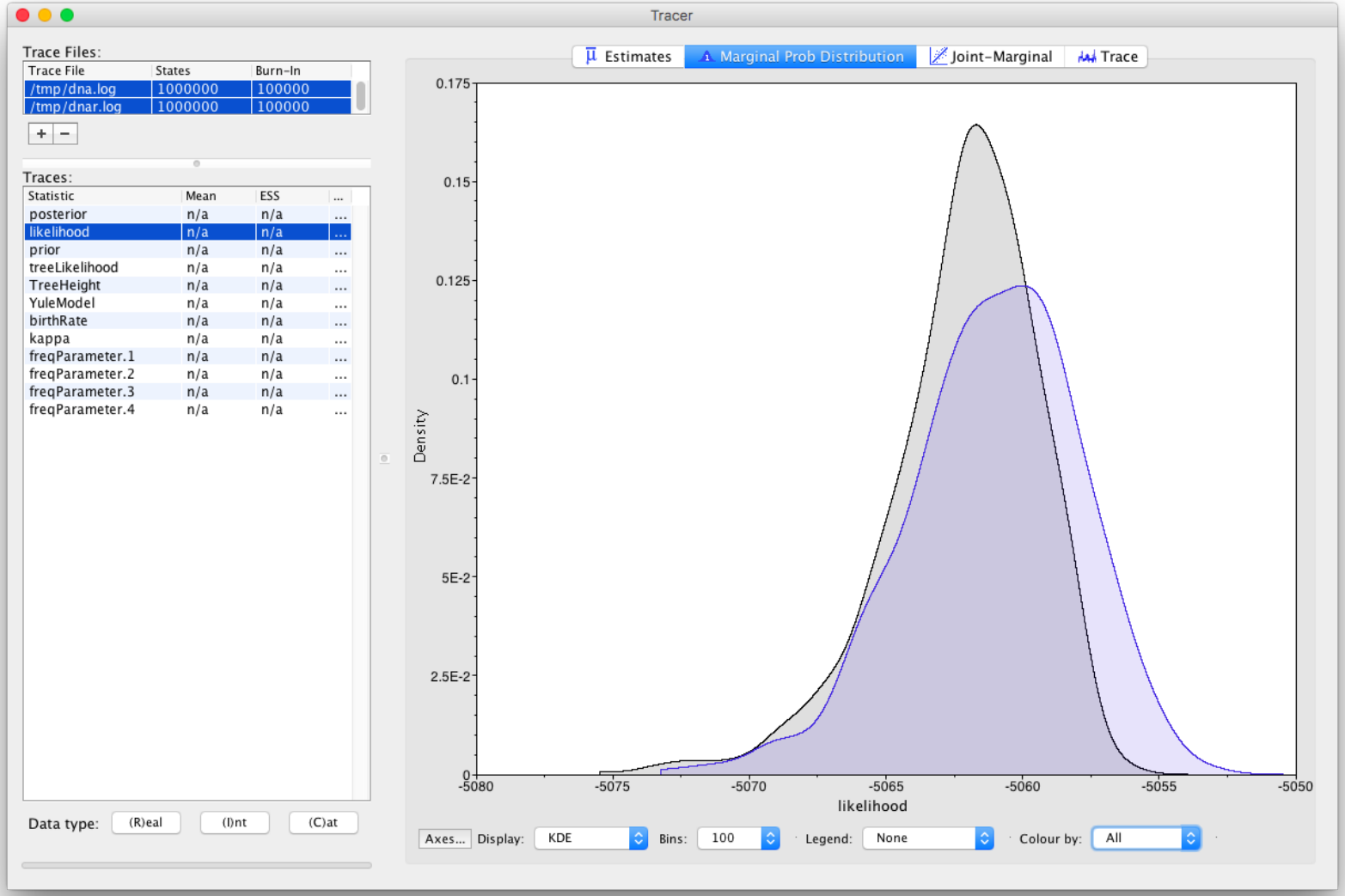
$$p(D|M) = \int_{\theta\in\Theta} \pi(\theta|M)L(D|M,\theta)d\theta$$

integrate/marginalise out θ

Bayes factor:

$$\frac{p(D|M_1)}{p(D|M_2)}$$

Model selection: "marginal likelihood" in Tracer



This is the likelihood averaged over samples from the posterior, not prior.

Model selection: marginal likelihood

Naive: Harmonic mean estimator (HME) of marginal likelihood

$$HME = \left(\frac{1}{n} \sum_{i=1}^{n} \frac{1}{L(D|\theta_i)} \right)^{-1}$$

where $\theta_1, \ldots, \theta_n$ a sample from the posterior

- Only requires a sample from the posterior
- Conveniently & quickly calculated in Tracer
- High variance estimator $\Rightarrow$ unreliable

Model selection: marginal likelihood

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- High variance estimator $\Rightarrow$ unreliable
- A post on Dr. Radford Neal's blog `http://radfordneal.wordpress.com/2008/08/17/the-harmonic-mean-of-the-likelihood-worst-monte-carlo-method-ever`

  "The total unsuitability of the harmonic mean estimator should have been apparent within an hour of its discovery."
- Never do this!

AICM model selection

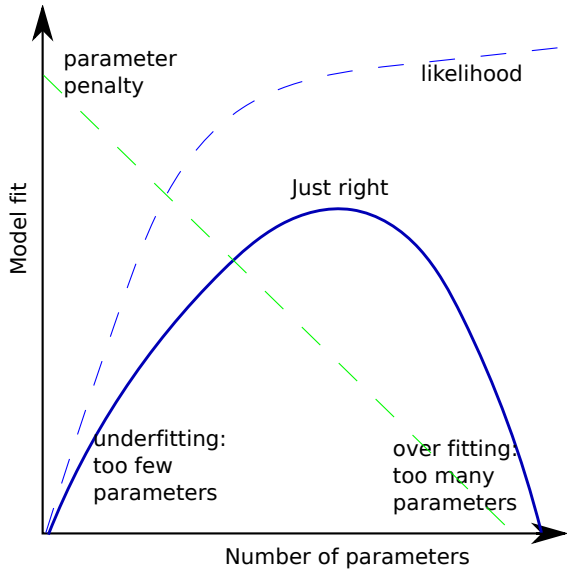
Akaike Information Criterion (AIC) by MCMC (AICM)

AIC:

$$2k - 2\log L(D|\theta)$$

k = effective number of parameters

$P(D|\theta)$ = likelihood



- Estimate k from fitting gamma distribution to MCMC sample of likelihood
- Smaller AICM is better (unlike marginal likelihood)
- Conveniently calculated in Tracer (or by model-selection package)

Path sampling/Stepping stone theory

- Marginal likelihood:

$$p(D) = \int_{\theta} \pi(\theta) L(D|\theta) d\theta$$

  hard to estimate directly.

- Define *power posterior* for some tractable reference distribution $p_w(\theta)$

$$P_\beta(\theta|D) = \frac{[L(D|\theta)\pi(\theta)]^\beta p_w(\theta)^{1-\beta}}{c_\beta}$$

  $P_1(\theta|D)$ is the posterior, c_1 the marginal likelihood.
  $P_0(\theta|D)$ is the reference distribution, $c_0 = 1$

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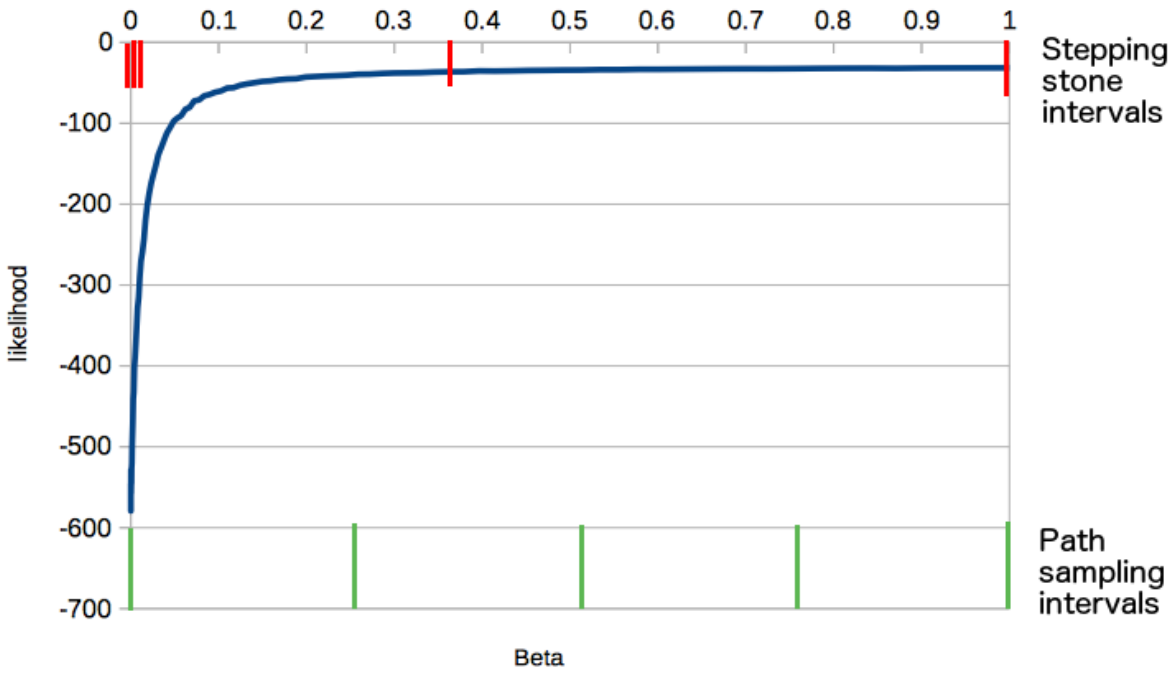
- $$\frac{c_{\beta_k}}{c_{\beta_{k-1}}} \approx \frac{1}{n} \sum_{i=1}^{n} p(D|\theta_{k-1,i})^{\beta_k - \beta_{k-1}}$$

- $$P(D|M) = \frac{c_1}{c_0} = \frac{c_1}{c_{0.3}} \frac{c_{0.3}}{c_{0.1}} \frac{c_{0.1}}{c_{0.01}} \frac{c_{0.01}}{c_0} = \frac{c_1}{\cancel{c_{0.3}}} \frac{\cancel{c_{0.3}}}{\cancel{c_{0.1}}} \frac{\cancel{c_{0.1}}}{\cancel{c_{0.01}}} \frac{\cancel{c_{0.01}}}{c_0}$$

Model selection: *Stepping stone* vs *path sampling*

Both use prior as reference distribution ($p_w(\theta) = \pi(\theta)$)



Stepping stone uses different intervals (set of β values) from path sampling, but otherwise the same

Generalised Stepping Stone

Use 'working distribution' for $p_w(\theta)$ based on posterior sample

- For parameters, use empirical distribution based on kernel estimators
- For trees, we need a distribution on topology and branch lengths

- Promises lower variance estimates
- Currently tedious to set up, since working distribution needs to be specified

Holder et al, Bayesian phylogenetics, 2014, Beale et al, Sys Bio, 2016

Pairwise Stepping Stone

Use posterior of M_2 for $p_w(\theta)$.

- Calculates Bayes factor between M_1 and M_2 directly
- $+$ requires fewer steps for accurate estimate
- – does not result in marginal likelihoods directly

Baele et al, BMC Bioinformatics, 2013

Path sampling/Stepping stone in practice

Number of steps:

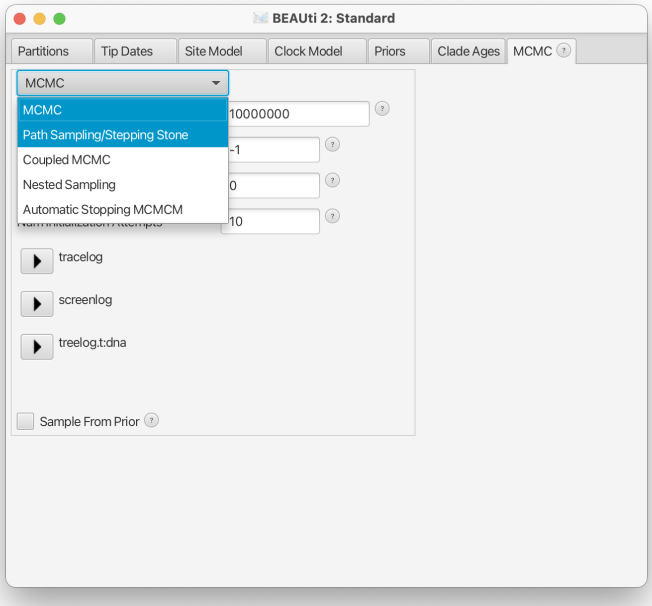
- Start with small nr of steps, say 16 and estimate ML
- increase nr of steps, estimate ML
- continue till ML estimate does not decrease any more

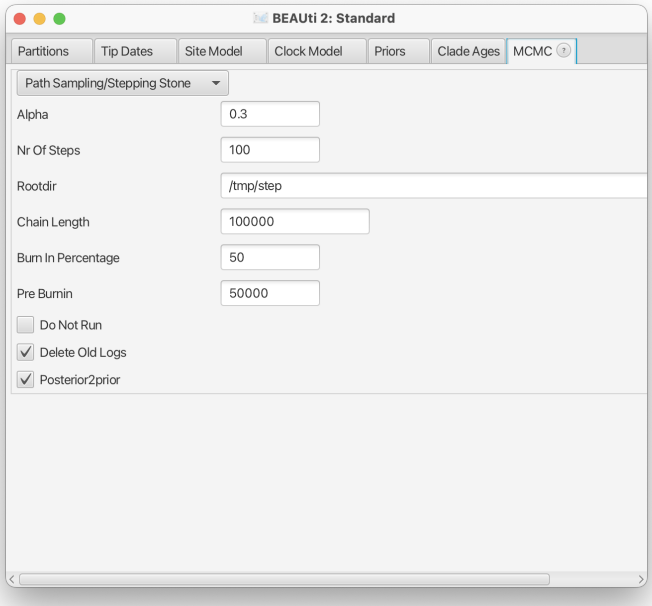
Chain length per step/ESS:

- total chain length at least as long as for posterior
- not all ESSs have to be 200 (errors cancel out)
- run different runs to get impression of variance of estimate
- use logcombiner to combine logs, for final estimate

Path sampling/Stepping stone in practice

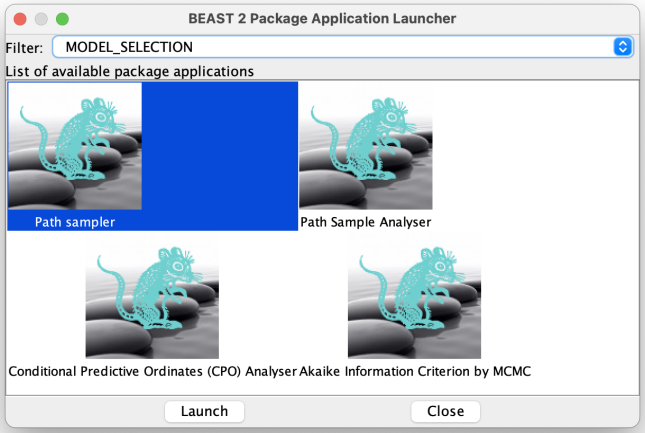
Requires MODEL_SELECTION package

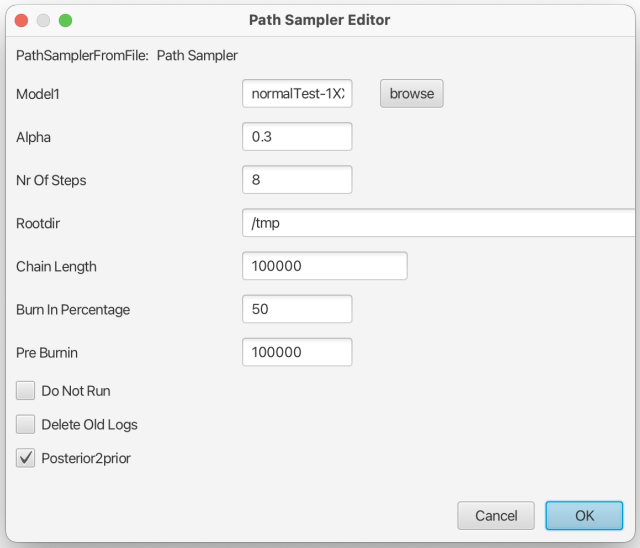




Path sampling/Stepping stone in practice

Set up through XML or GUI





Set up through CLI:

- to list BEAST apps:
  `/path/to/applauncher -list`
- To show `PathSampler` options:
  `/path/to/applauncher PathSampler -help`
- To set up `PathSampler` analysis:
  `/path/to/applauncher PathSampler -nrOfSteps 64 -rootdir dir/withs/steps -burnInPercentage 50 -model beast.xml`

Path sampling/Stepping stone in practice

To set up on a HPC cluster

- Set up locally, using 'doNotRun' flag = true
- Move steps to cluster, and run steps in paralel there
- Estimate ML using `PathSampleAnalyser`

```
/path/to/applauncher PathSampleAnalyser -nrOfSteps 64
-rootdir dir/withs/steps -burnInPercentage 50
```

Path sampling/Stepping stone in practice

Trouble shooting

- ESS too small for a step: resume runs for that step
- Infinite likelihoods caused by numeric instability: improper priors – use proper priors instead
- -Infinite likelihoods: priors too wide – narrow priors
- Inspect log files in step directory to see which parameter escapes, so which prior to adjust

Nested Sampling Theory

$$\mathcal{Z} = \int_{\theta} \pi(\theta) L(\theta) \mathrm{d}\theta$$

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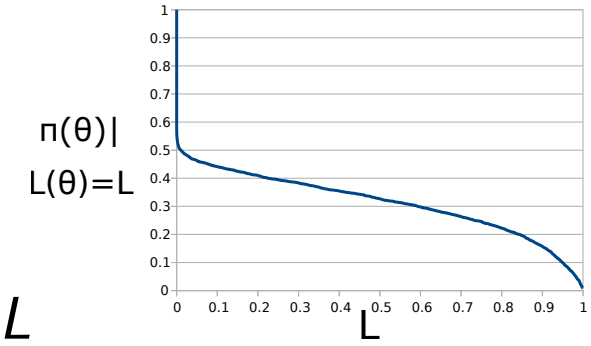
$$= \int_{L=0}^{\infty} L \left(\int_{\theta, L(\theta)=L} \pi(\theta) \mathrm{d}\theta \right) \mathrm{d}L$$



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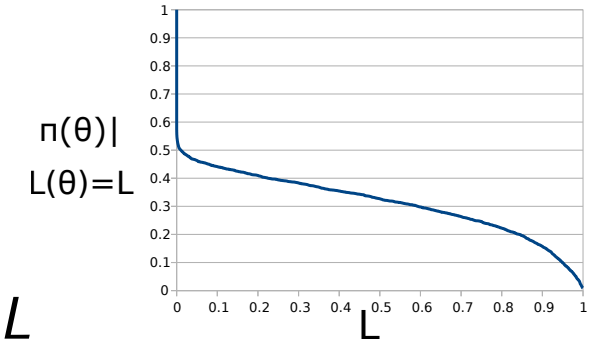
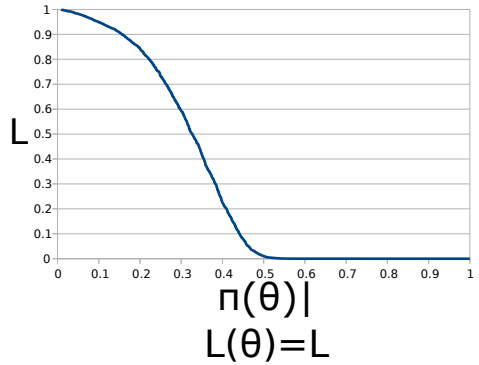
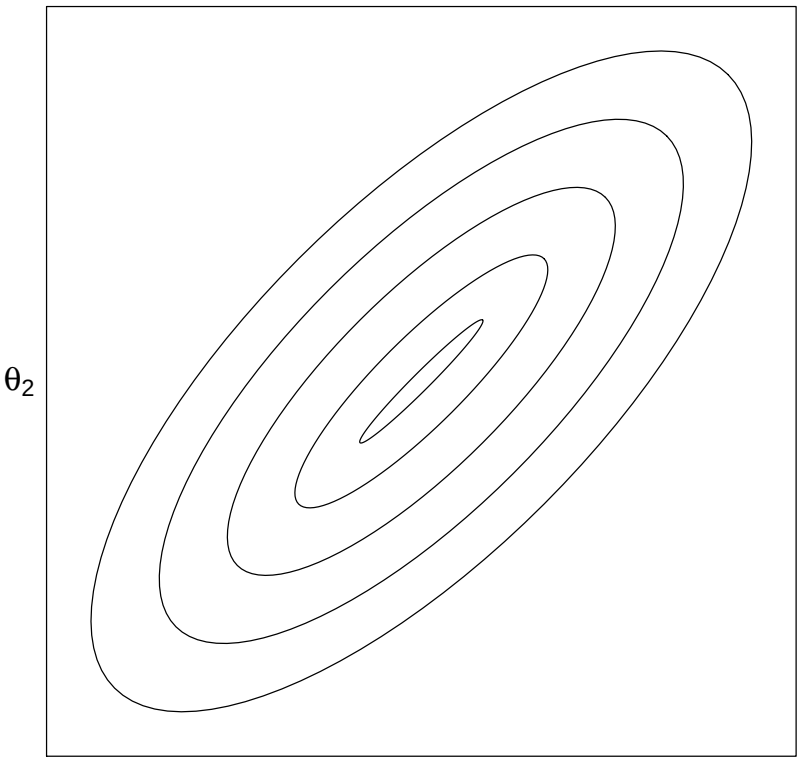


$$= \int_{X=0}^{1} \mathcal{L}(X) \mathrm{d}X$$

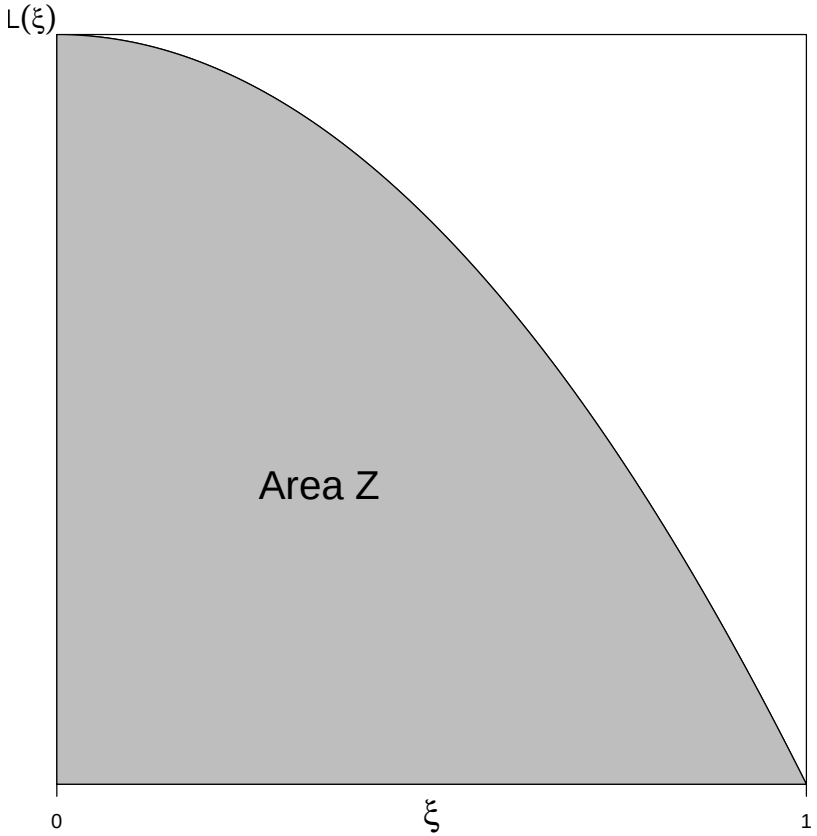


where $\mathcal{L}(X)$ inverse likelihood

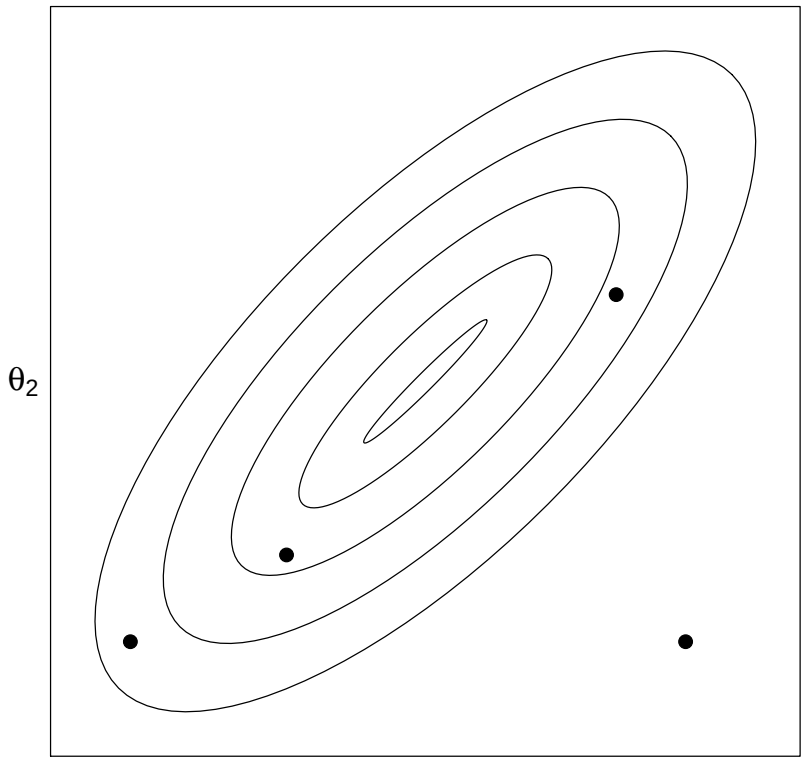
Nested sampling



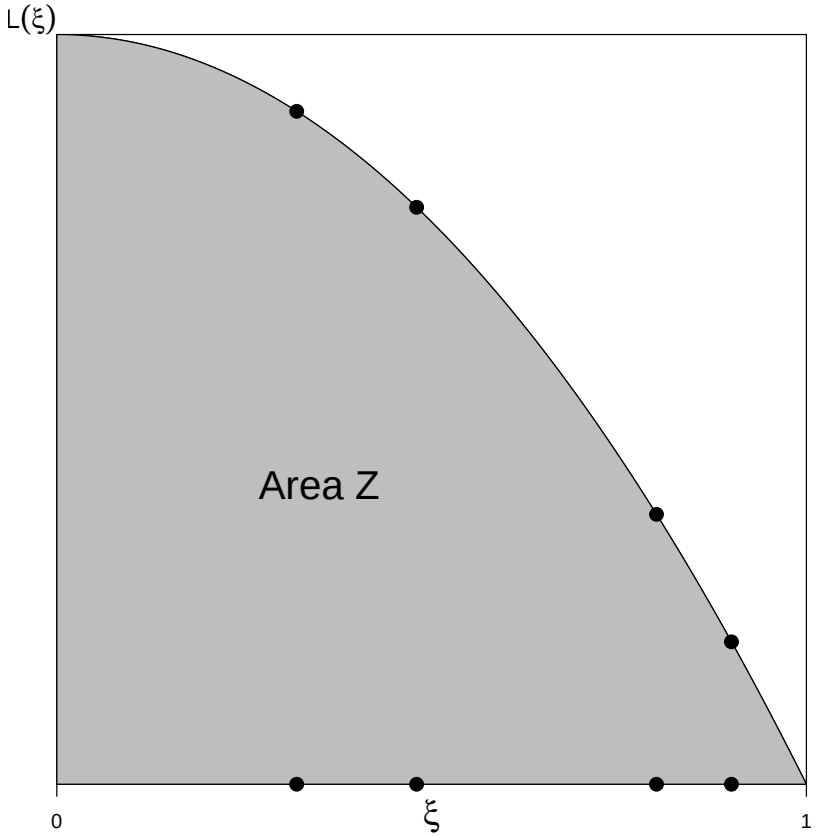
images courtesy Patricio Russell



Nested sampling



images courtesy Patricio Russell



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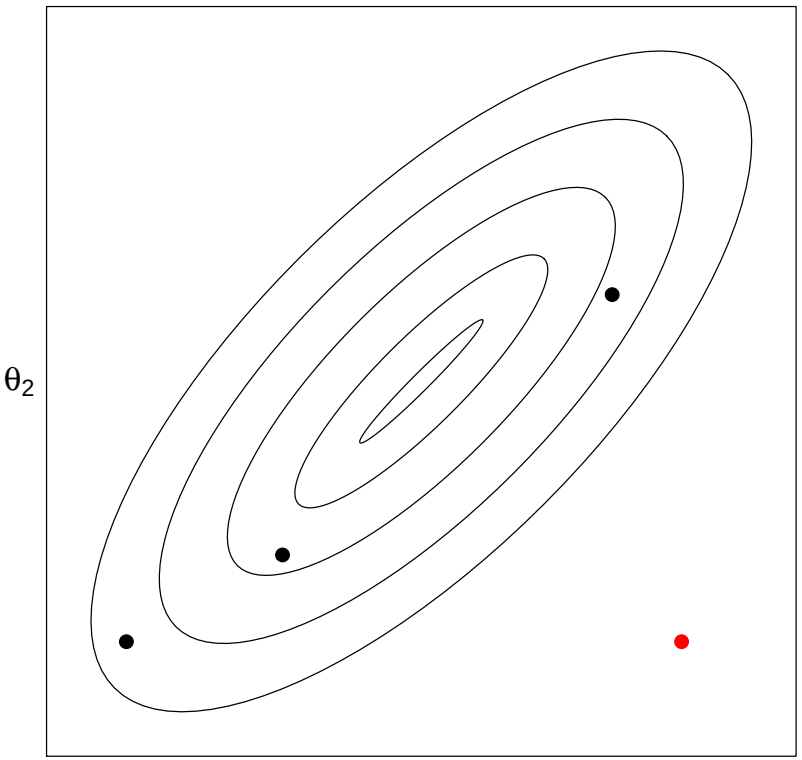

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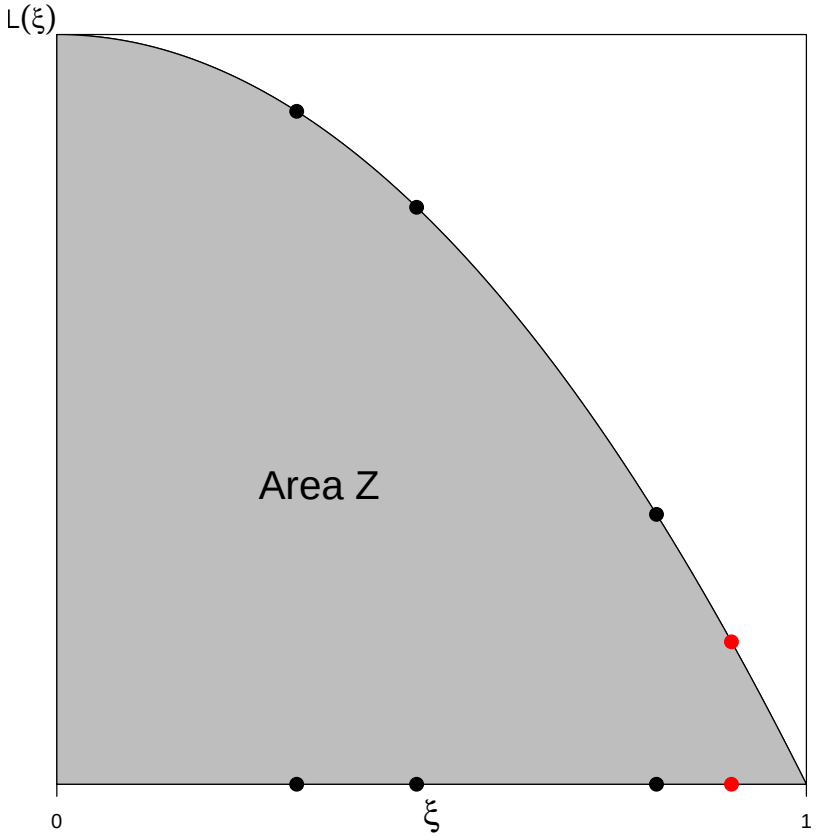

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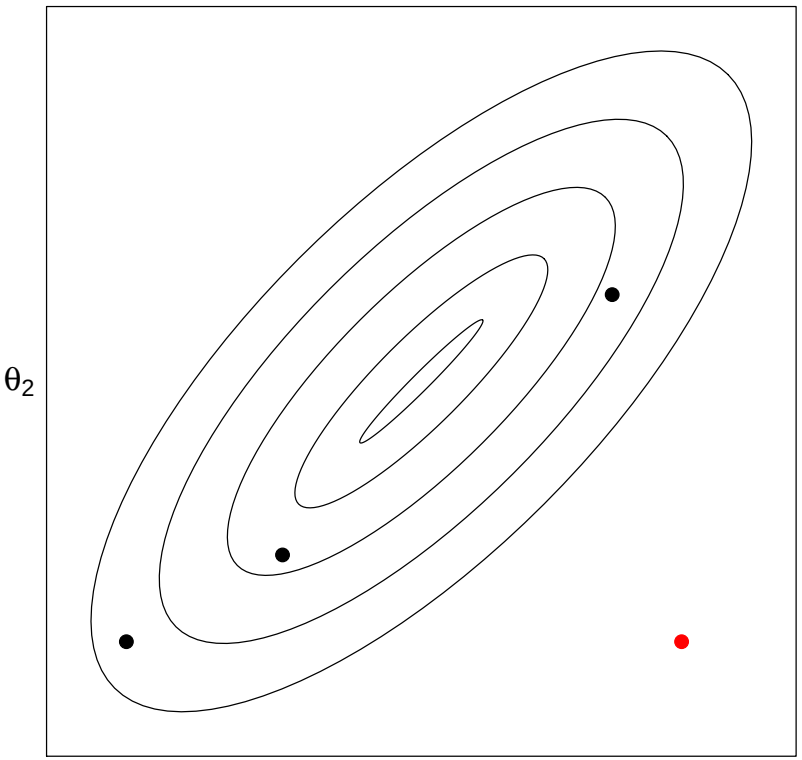

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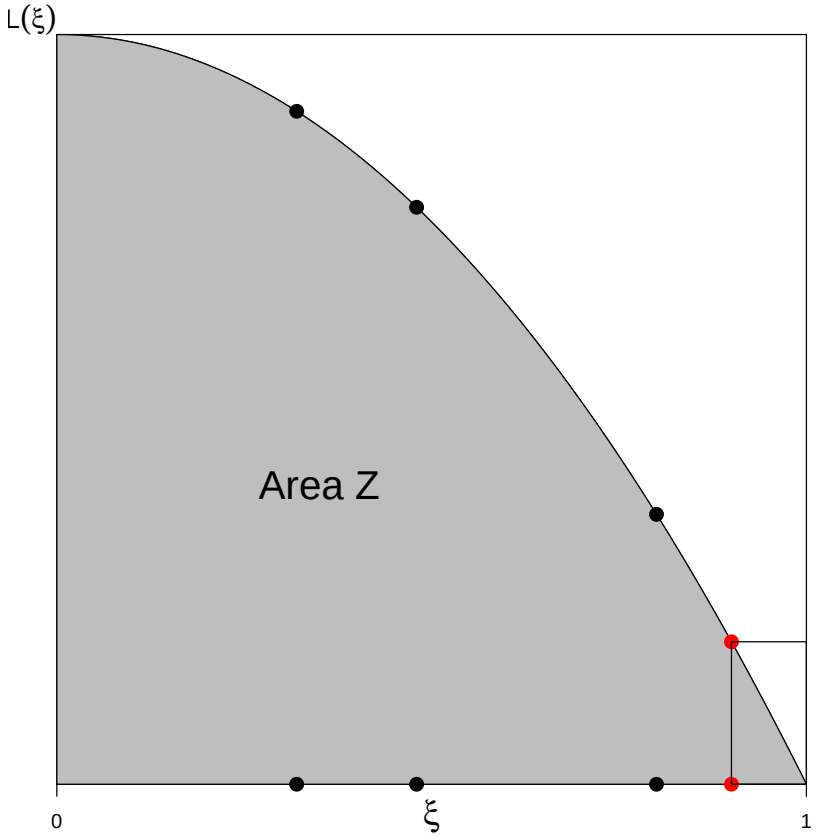

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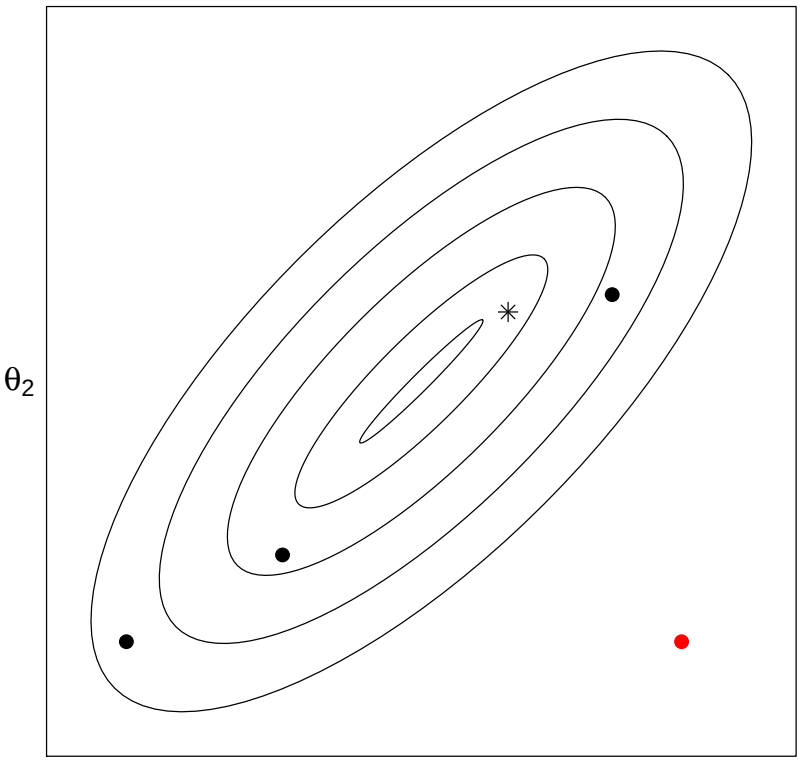

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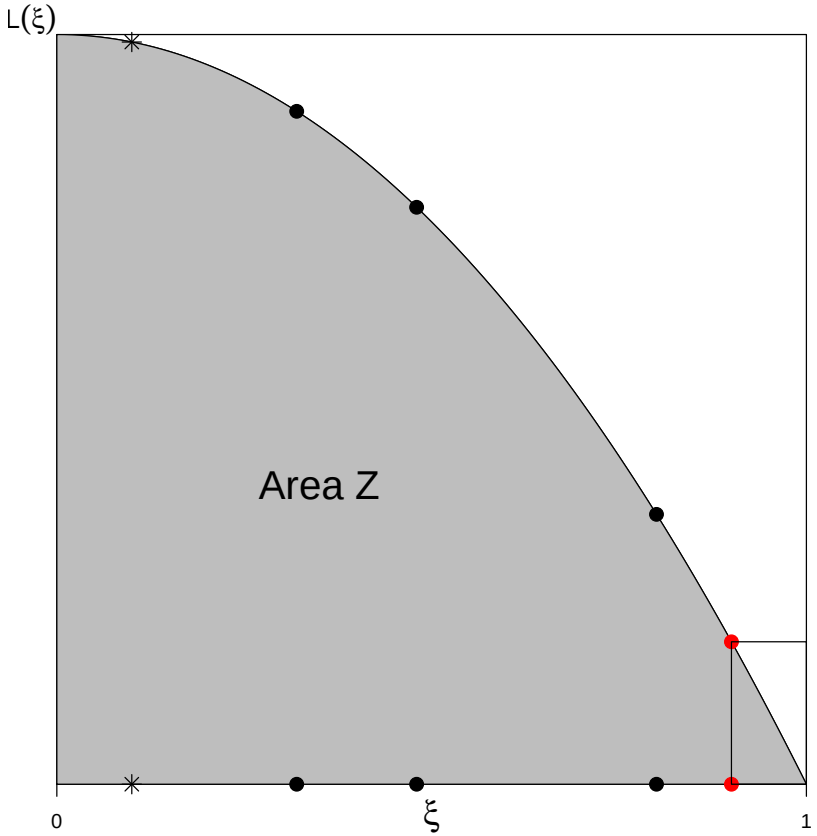

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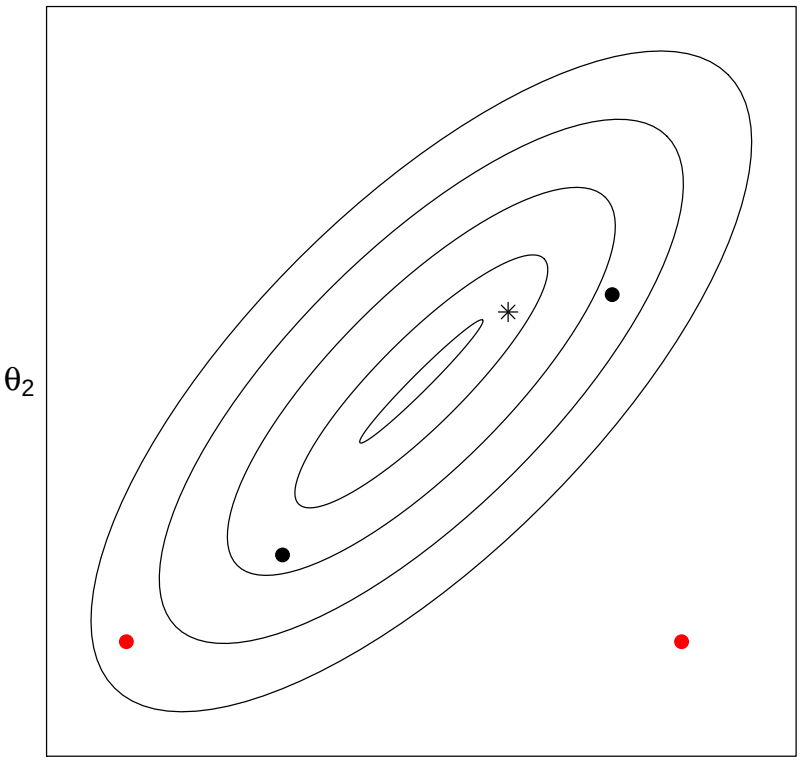
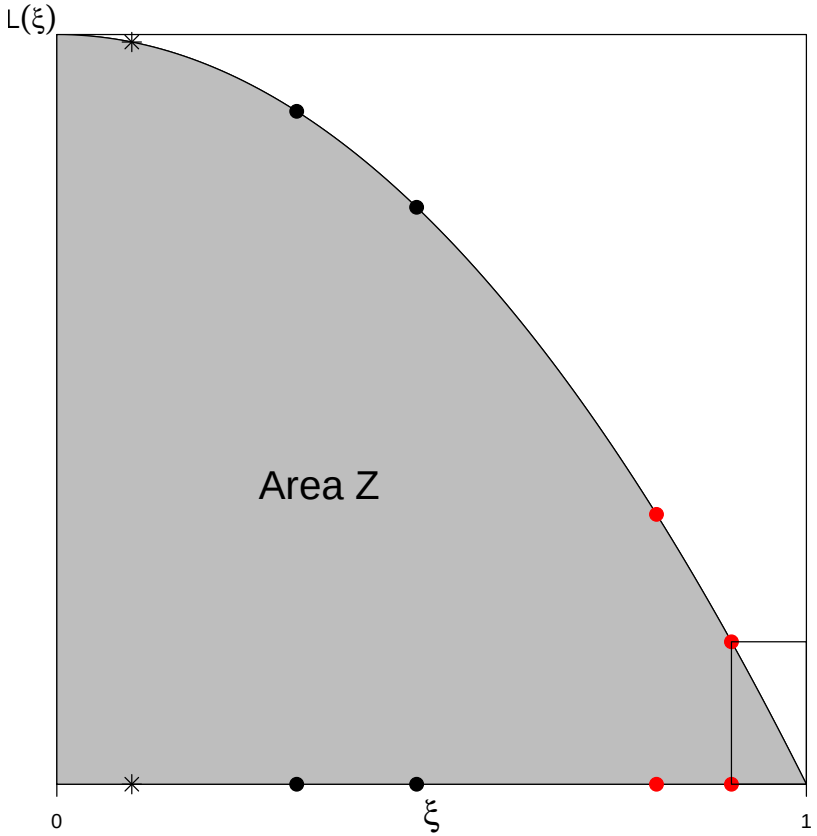


images courtesy Patricio Russell



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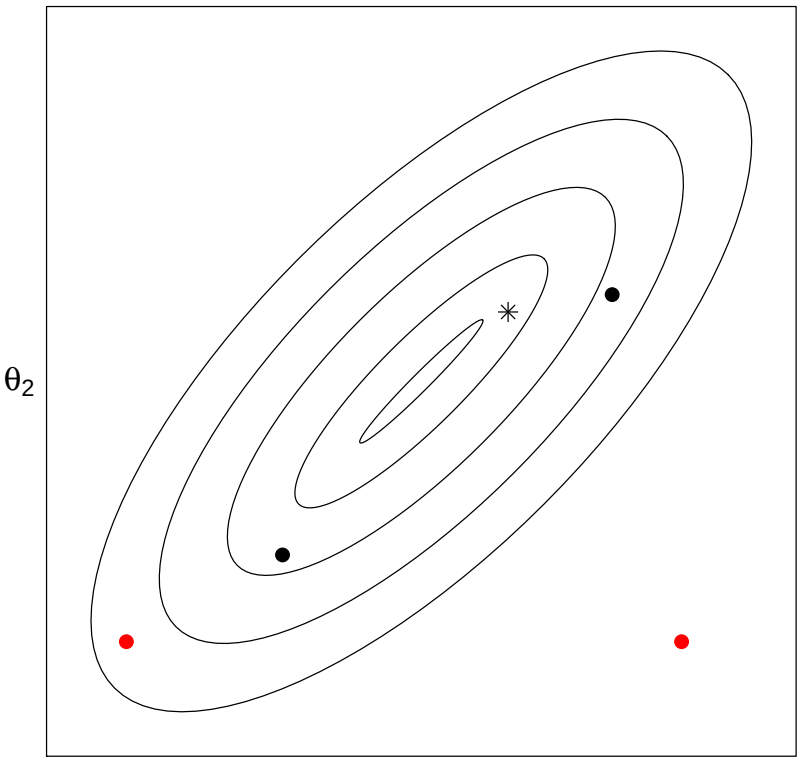

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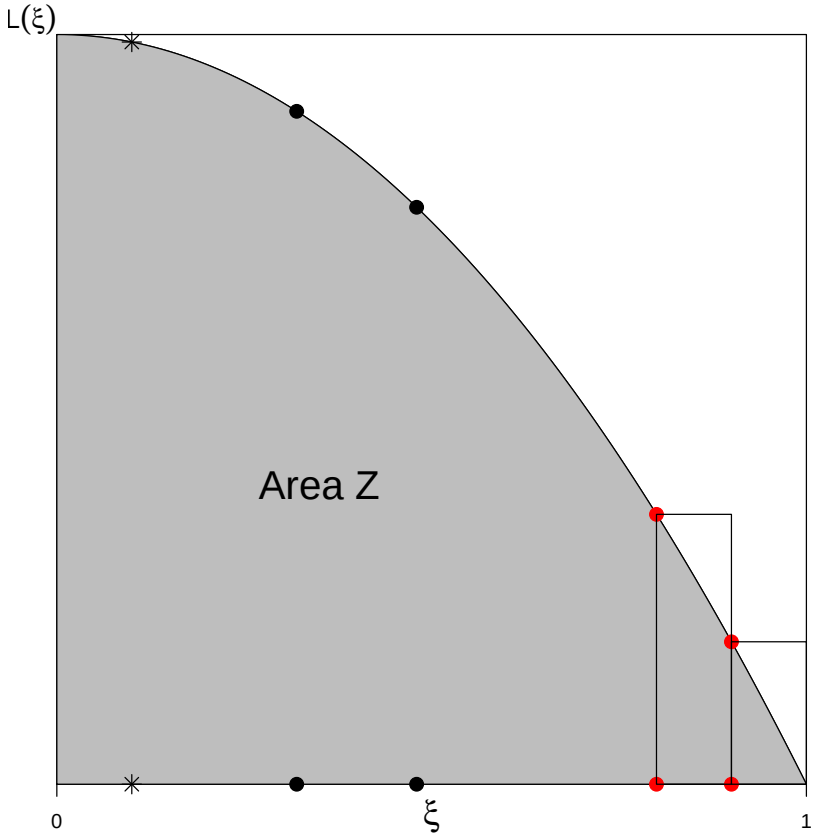

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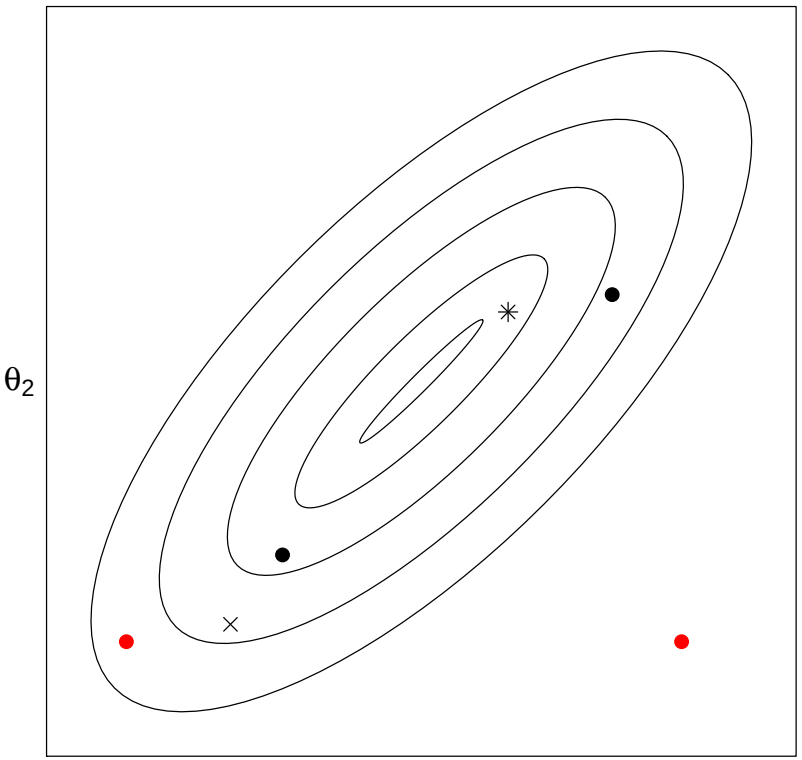
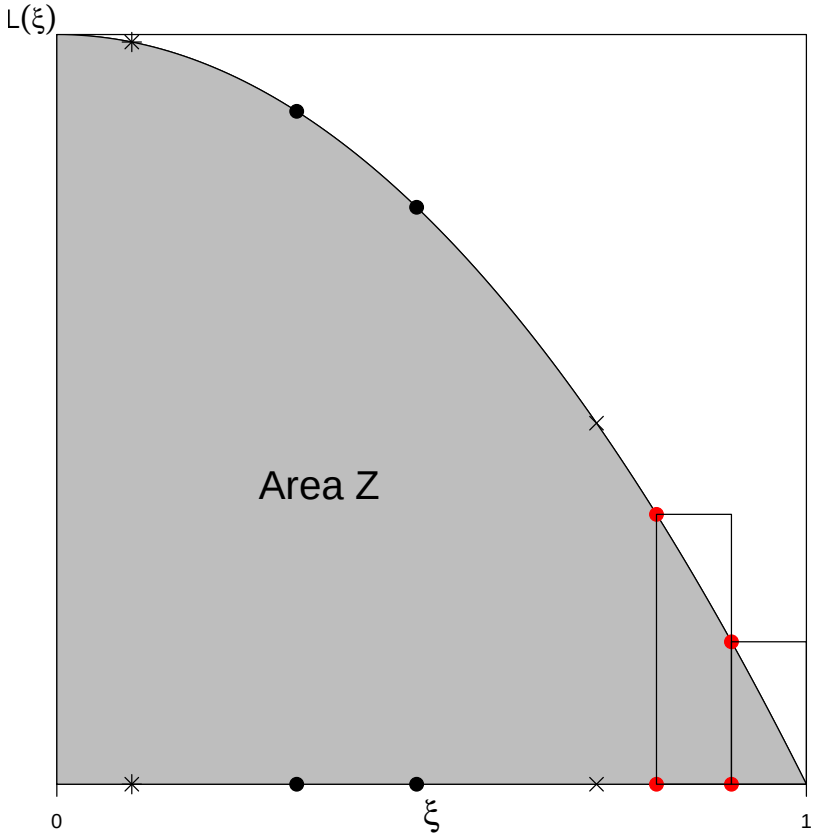


images courtesy Patricio Russell



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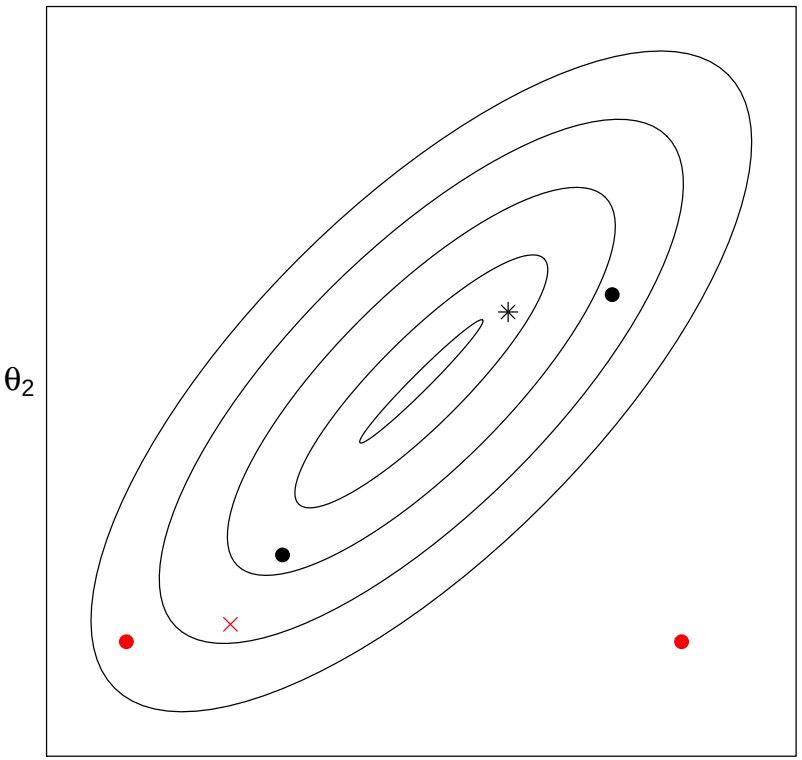
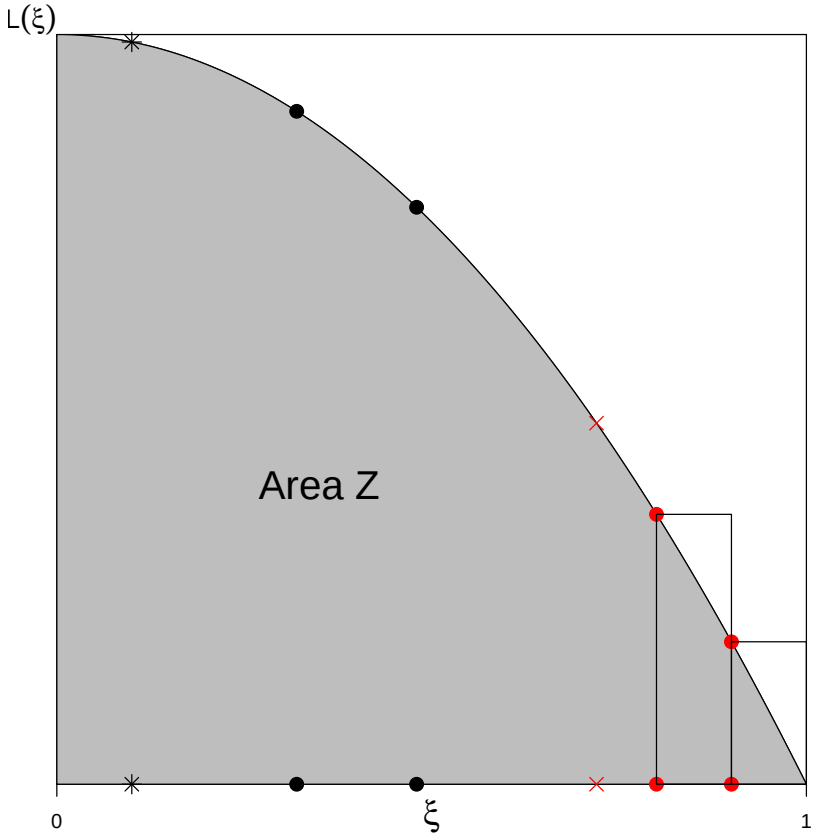
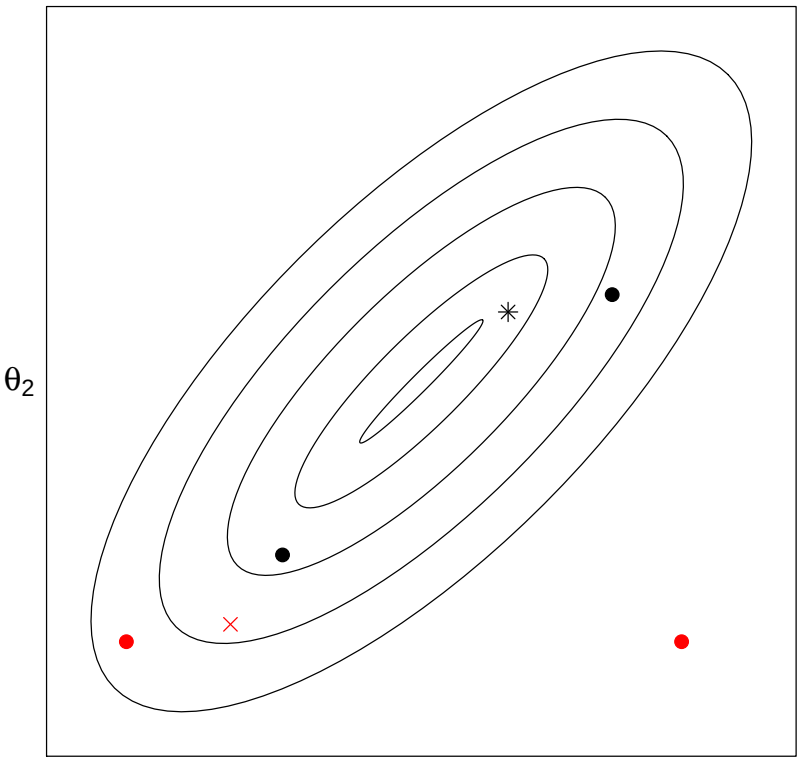


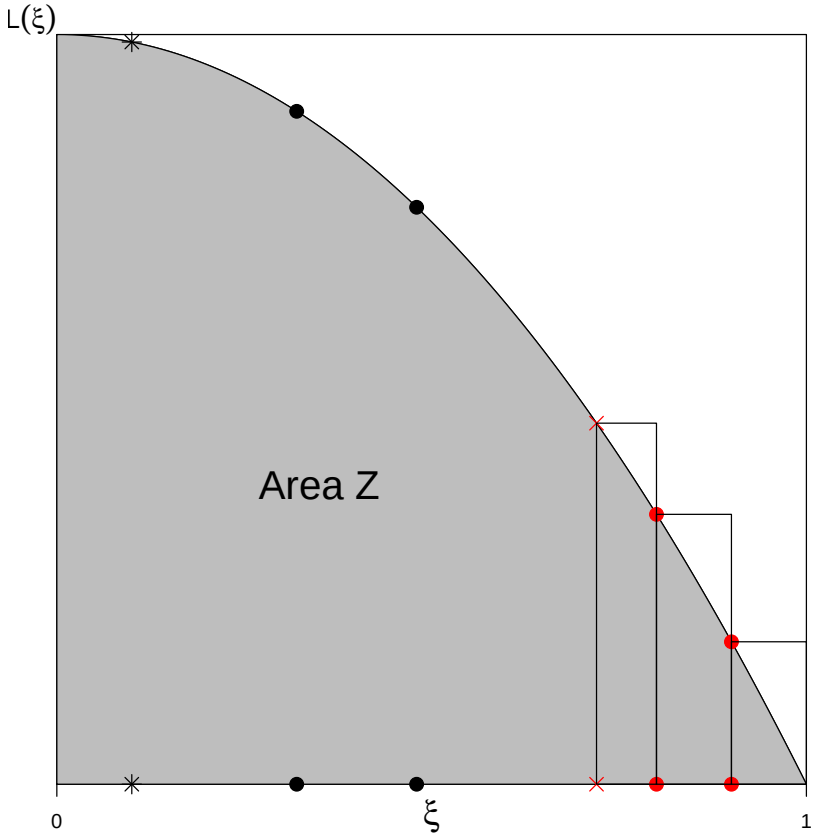
images courtesy Patricio Russell



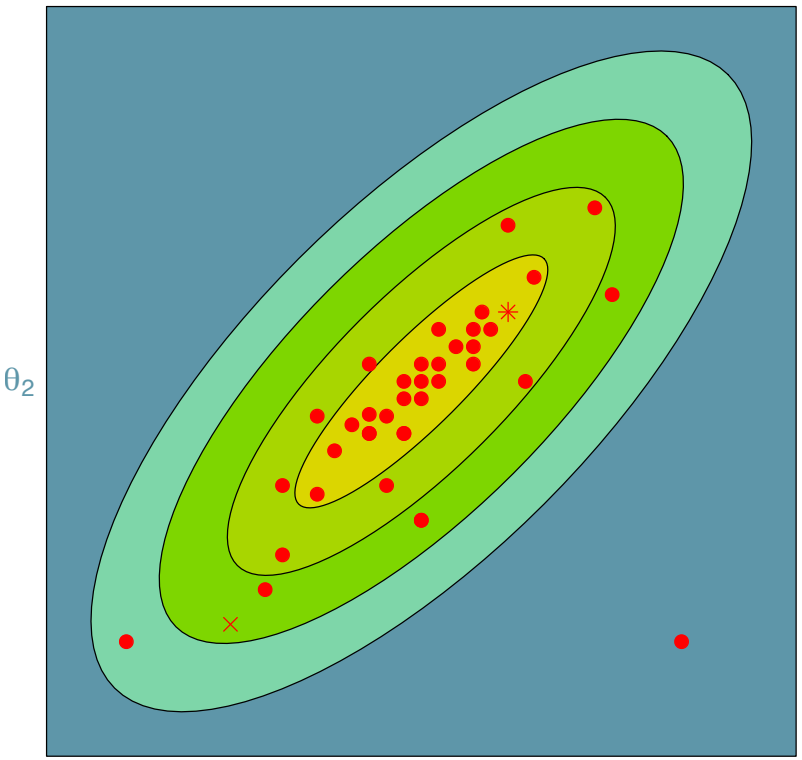
Nested sampling

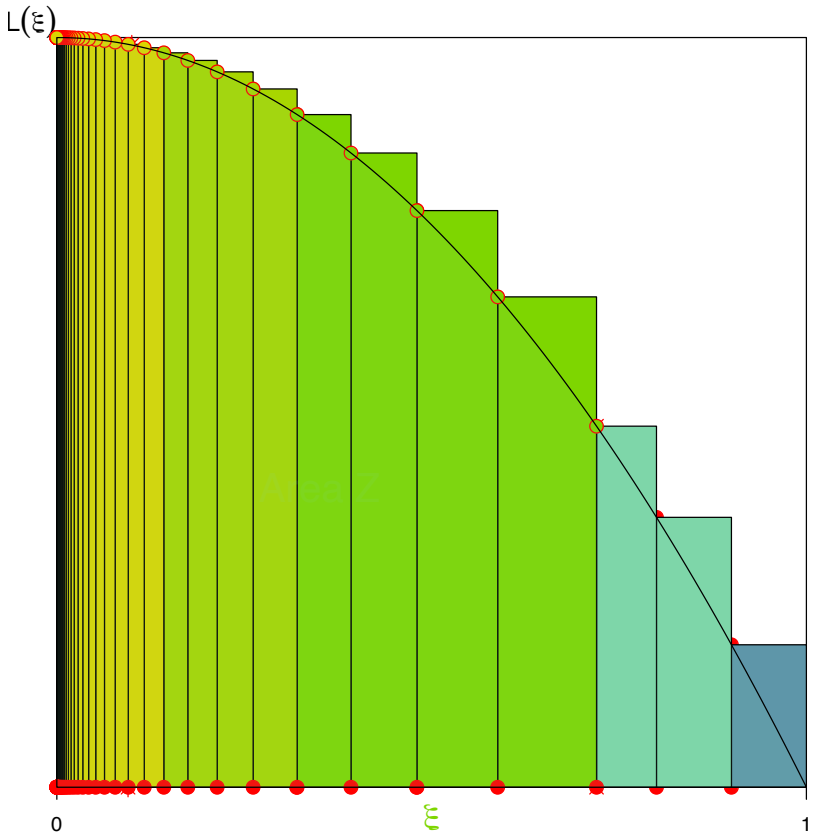


images courtesy Patricio Russell



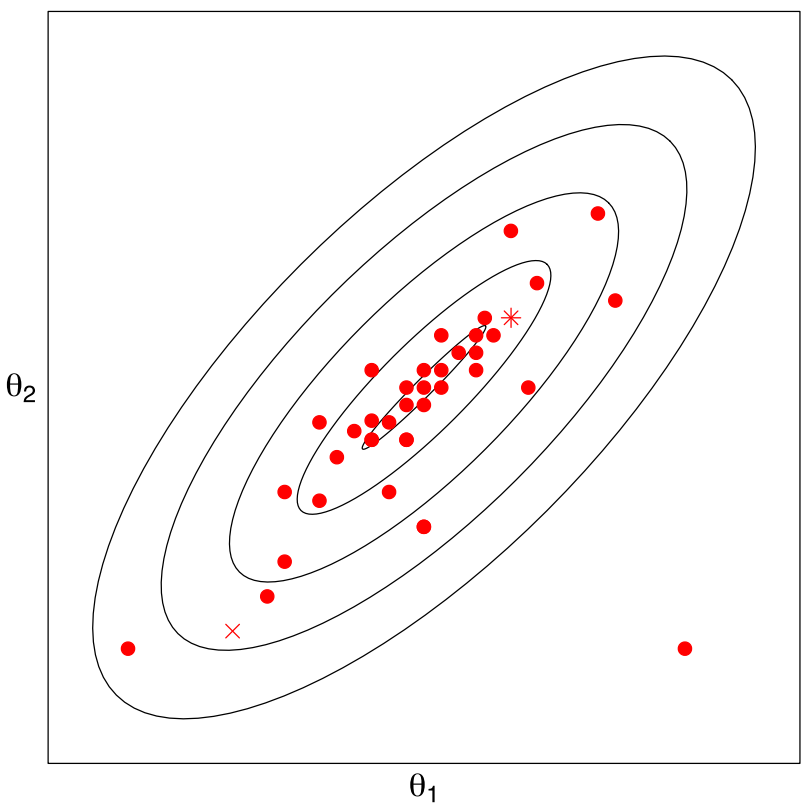
Nested sampling

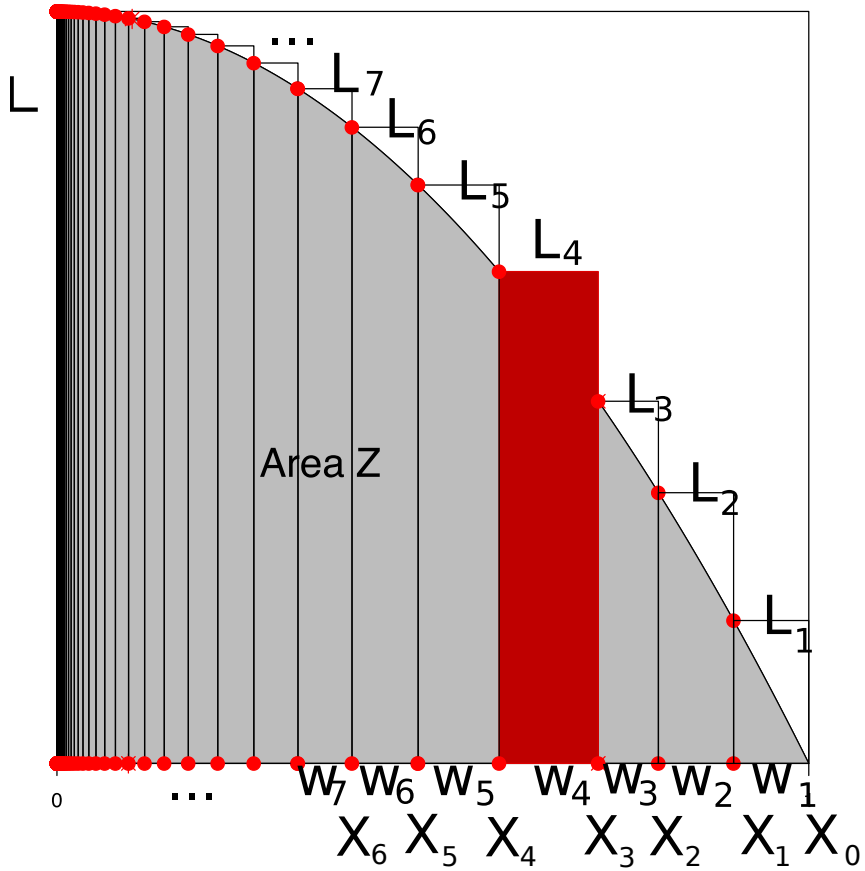




images courtesy Patricio Russell

Area under curve is ML $= \mathcal{Z}$, with N active points





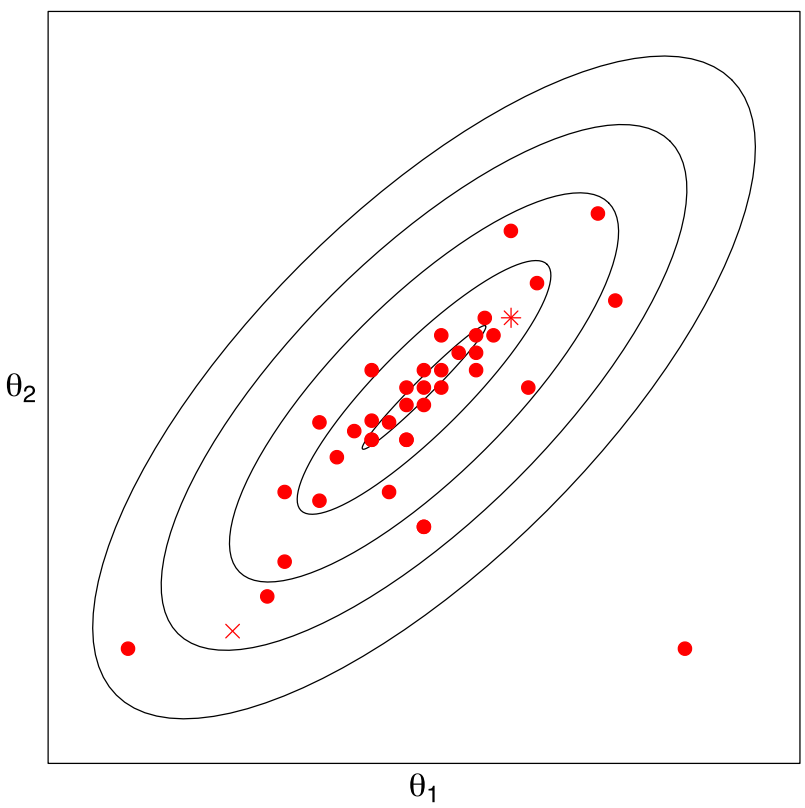
$X_0 = 1$

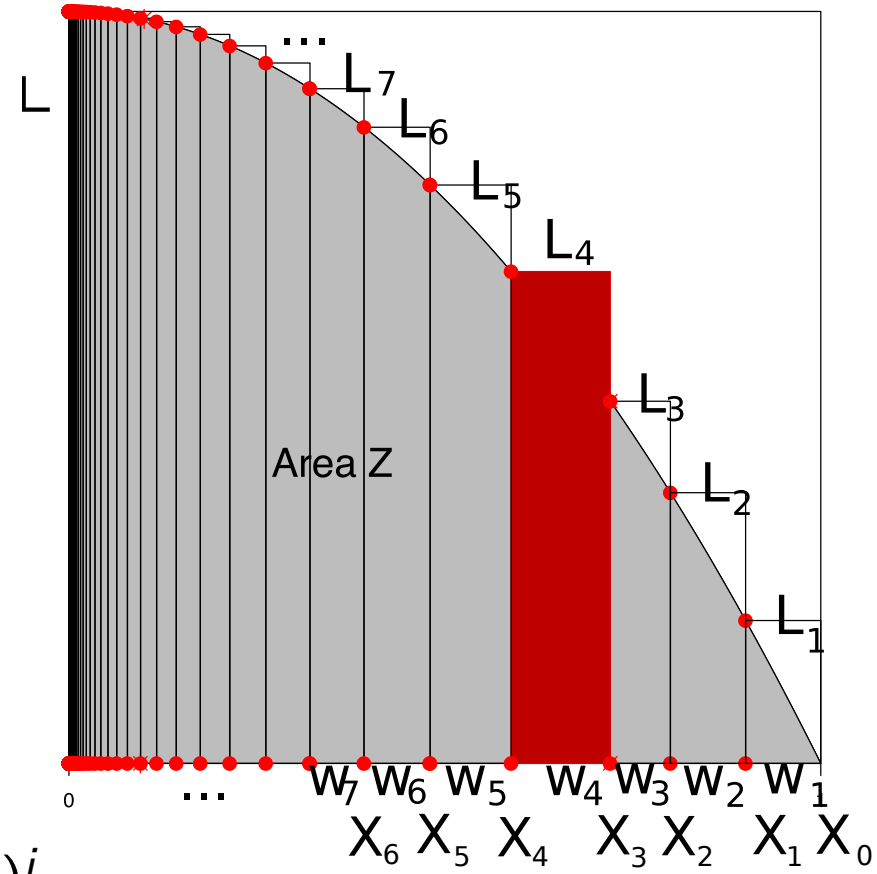
$X_i =$ proportion of prior mass with likelihood at least L_i

$w_i = X_i - X_{i-1}$

$\mathcal{Z} \approx \sum_i w_i L_i$

Defining X_i with N active points

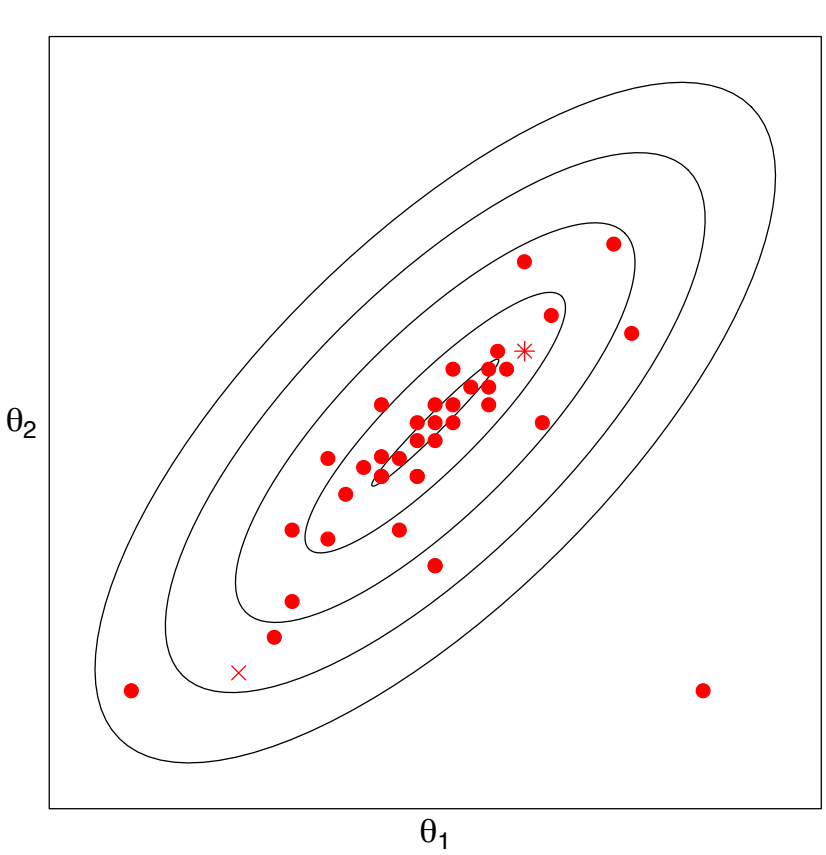


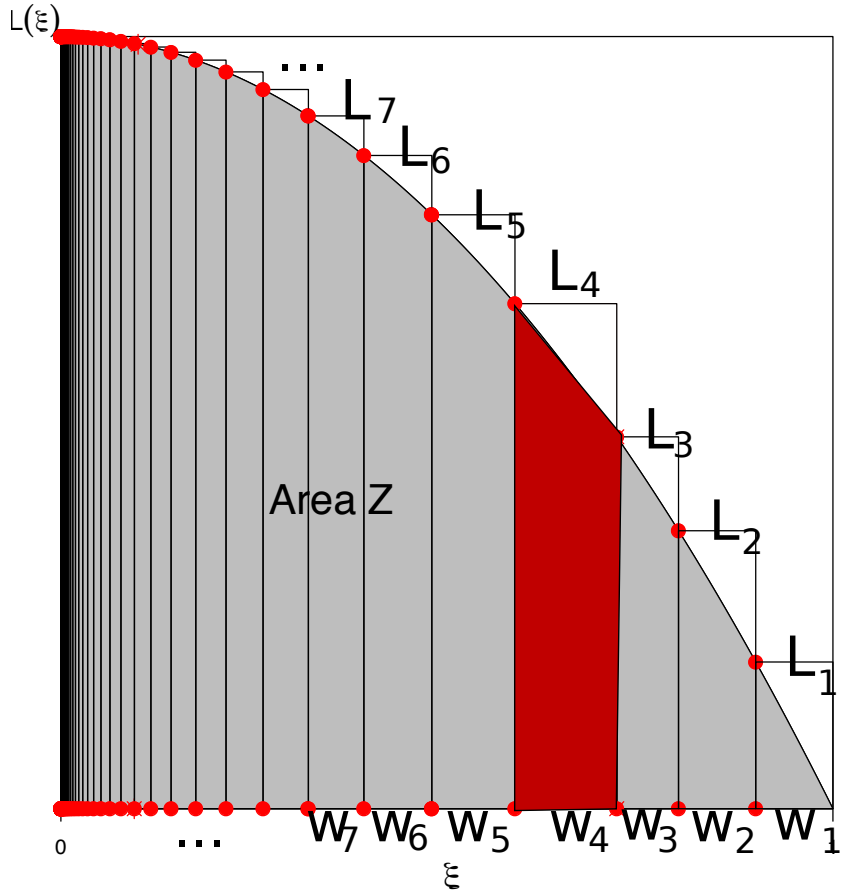


1. Arithmetic mean: $X_i = (\frac{N}{N+1})^i$
2. Geometric mean: $X_i = e^{-\frac{i}{N}}$ <= fast, most popular
3. Stochastic: $X_i = \beta(1, N)X_{i-1}$, $X_0 = 1$ <= allows SD estimate

$w_i = X_i - X_{i-1}$ $\qquad$ $\mathcal{Z} \approx \sum_i w_i L_i$

Use trapezium rule for more accurate ML estimate





$$\mathcal{Z} = \sum \ldots$$

Nested sampling with N active points

Assign weights to 'saved points'

$$E\{w_i\} = e^{-(i-1)/N} - e^{-i/N}$$

Estimate of marginal likelihood

$$\mathcal{Z} = \sum_i w_i L_i$$

Nested sampling with N active points

Assign weights to 'saved points'

$$E\{w_i\} = e^{-(i-1)/N} - e^{-i/N}$$

Estimate of marginal likelihood

$$\mathcal{Z} = \sum_i w_i L_i$$

Estimate of standard deviation of marginal likelihood

$$sd(\log \mathcal{Z}) = \sqrt{\frac{H}{N}}$$

where the information $H \approx \sum_i w_i \frac{L_i}{\mathcal{Z}} log \frac{L_i}{\mathcal{Z}}$

Nested sampling with N active points

Assign weights to 'saved points'

$$E\{w_i\} = e^{-(i-1)/N} - e^{-i/N}$$

Estimate of marginal likelihood

$$\mathcal{Z} = \sum_i w_i L_i$$

Estimate of standard deviation of marginal likelihood

$$sd(\log \mathcal{Z}) = \sqrt{\frac{H}{N}}$$

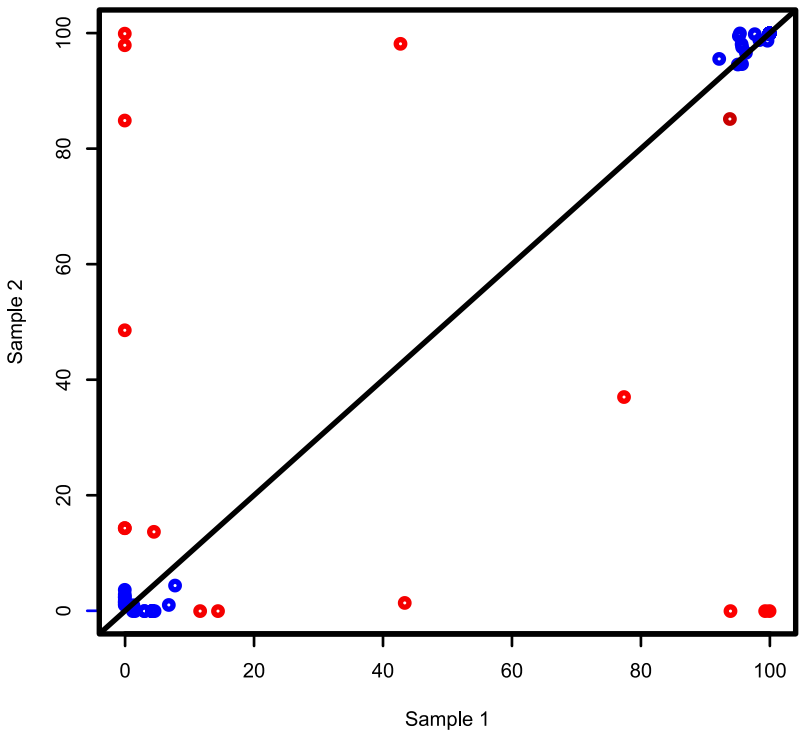
where the information $H \approx \sum_i w_i \frac{L_i}{\mathcal{Z}} log \frac{L_i}{\mathcal{Z}}$

Sample from posterior by sampling saved points according to weights $\frac{w_i L_i}{\mathcal{Z}}$

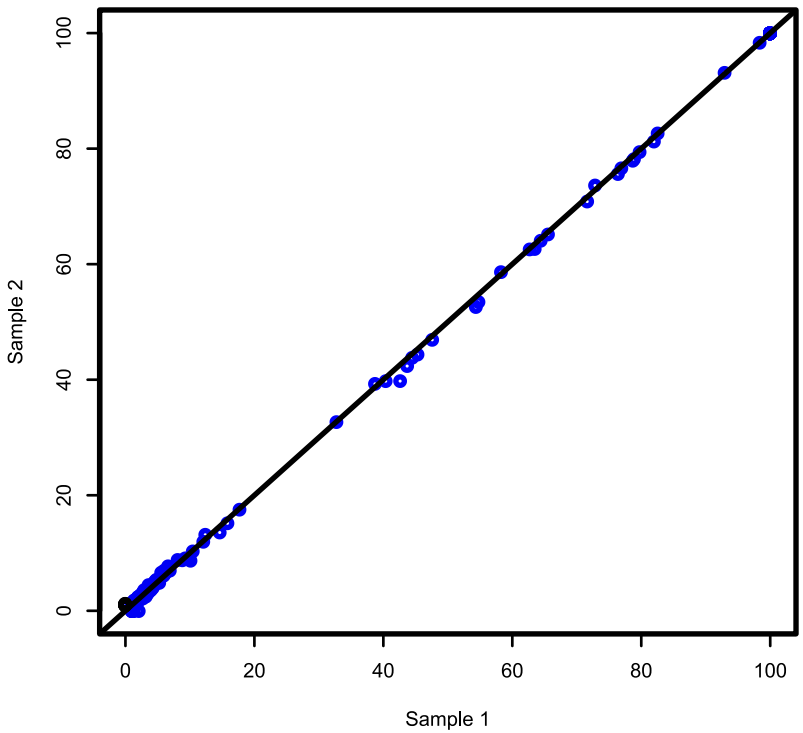
DS1: where MCMC fails

- DS1 data set with tree islands
- MCMC has trouble moving between islands
- Consequently MCMC/stepping stone/path sampling fails

MCMC

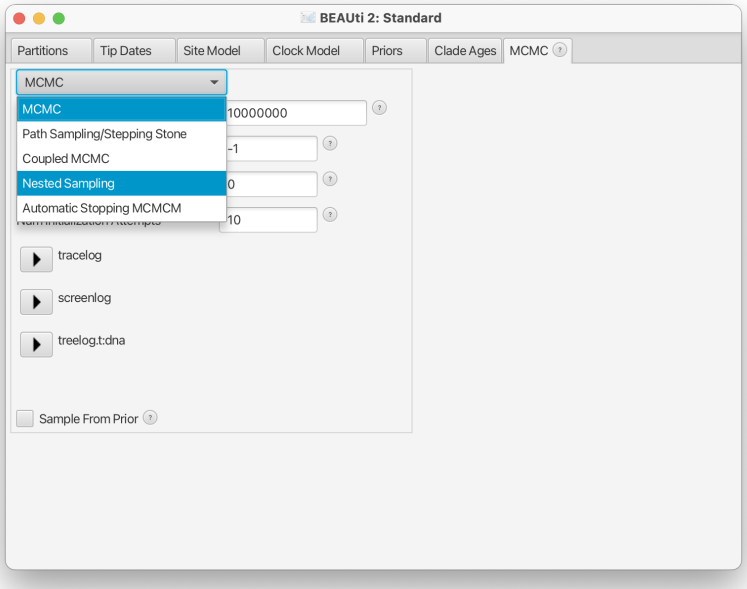


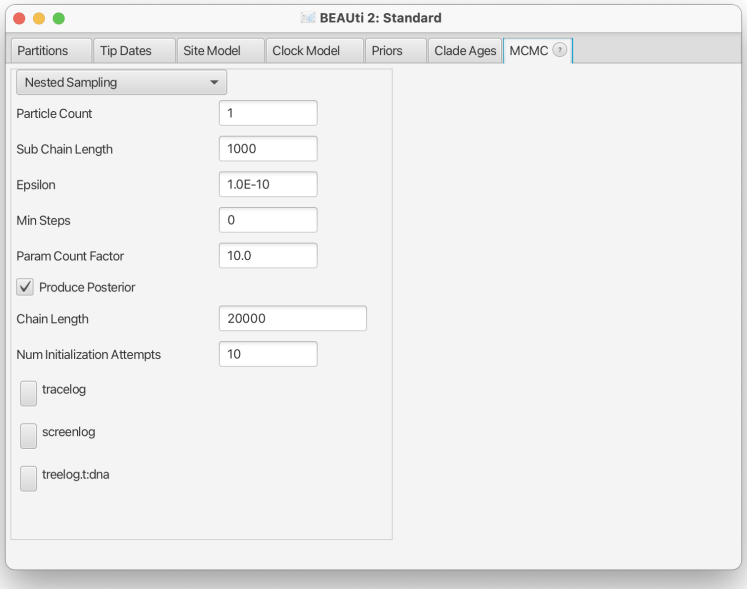
Nested sampling



NS in practice: Setting up an analysis

Requires NS package





NS in practice: Setting up an analysis

Set up analysis in BEAUti, then edit XML and replace

```
<run id="mcmc" spec="MCMC" chainLength="100000000">
```

with

```
<run id="mcmc" spec="beast.gss.NS" chainLength="20000"
   particleCount="1" subChainLength="5000" epsilon="1e-12">
```

More info:
https://github.com/BEAST2-Dev/nested-sampling/wiki/How-to-use-NS

NS in practice: Are we there yet?

- Run multiple times (like MCMC).
- Check $\mathcal{Z}$ estimates are compatible

$$|\log \mathcal{Z}_1 - \log \mathcal{Z}_2| \leq 2\sqrt{(SD_1^2 + SD_2^2)}$$

- If not, run with longer sub chain length
- Check $\mathcal{Z}$ estimates are compatible with shorter runs/not systematically biased in multiple runs

Note, nested sampling under estimates $\mathcal{Z}$. Longer sub chain length results in lower $\mathcal{Z}$ if not converged yet.

NS in practice: Model selection with Nested sampling

Given M_1 and M_2: say HKY vs GTR

1. estimate log marginal likelihoods $\mathcal{Z}_1$ for M_1 and $\mathcal{Z}_2$ for M_2
   • NS provides standard deviations SD_1 and SD_2 for **log** marginal likelihoods
2. if $|\log \mathcal{Z}_1 - \log \mathcal{Z}_2| \geq 2\sqrt{SD_1^2 + SD_2^2}$ calculate Bayes factor $BF = \log \mathcal{Z}_1 - \log \mathcal{Z}_2$. Done!
3. else if $\sqrt{SD_1^2 + SD_2^2} < 3(?)$ then M_1 and M_2 cannot be distinguished. Done!
4. else, run NS with more particles. How many? Use $SD = \sqrt{\frac{H}{N}}$ so $N = SD^2/H$ for desired SD (H from NS run) and goto (2)

NS in practice: Pitfalls

- Subchain length too short – run with different length, compare whether estimates differ
- Epsilon too large, causing early stopping, underestimate of $\mathcal{Z}$
- ...

NS in practice: Parallel implementation

- Maintaining shared pool to selected starting point => behaves like single thread N particle
- Runtime scales linear with nr or particles N
- N single particle runs can be combined => embarrassingly parallel
- Little communication required, so can be forked out over different CPUs

Stepping Stone and Nested Sampling work on any model

provided the prior is proper

Model selection summary

Stepping Stone and Nested Sampling work on any model

provided the prior is proper

Improper priors do not integrate to one, e.g., 1/X, uniform(0,∞)

Model selection summary

- Naive: Harmonic mean estimator (HME) of marginal likelihood
  - High variance estimator $\Rightarrow$ unreliable
  - Never do this!
- AICM: Akaike information criterion for MCMC
  - Computational convenient
  - High variance estimator $\Rightarrow$ unreliable (but better than HME)
  - only use when stepping stone/nested sampling is not feasible
- Path sampling/Stepping stone:
  - computationally expensive
  - most stable marginal likelihood estimation we got (so far)
  - use this if you can
- Nested sampling:
  - Provides estimate of ML + its variance
  - Computation (inverse) proportional to accuracy of estimate
  - Can choose accuracy as desired

Model comparison/Bayesian hypothesis testing

- Through model selection:
  - compare Bayes factors based on ML estimates
- Through model averaging: post-hoc analysis
  - compare Bayes factors based on empirical estimates from prior and posterior samples

Bayes factor:

$$\frac{p(D|M_1)}{p(D|M_2)} \text{ estimated by } \frac{\frac{empirical\ \ posterior(M_1)}{empirical\ \ prior(M_1)}}{\frac{empirical\ \ posterior(M_2)}{empirical\ \ prior(M_2)}}$$

Obtain sample from prior for M_1 and M_2.
Obtain sample from posterior for M_1 and M_2.

Bayes Factors

BF range			$\ln(BF)$ range			$\log_{10}(BF)$ range			Interpretation
1	–	3	0	–	1.1	0	–	0.5	hardly worth mentioning
3	–	20	1.1	–	3	0.5	–	1.3	positive support
20	–	150	3	–	5	1.3	–	2.2	strong support
	$>$	150		$>$	5		$>$	2.2	overwhelming support

Kass & Raftery, JASA, 1995

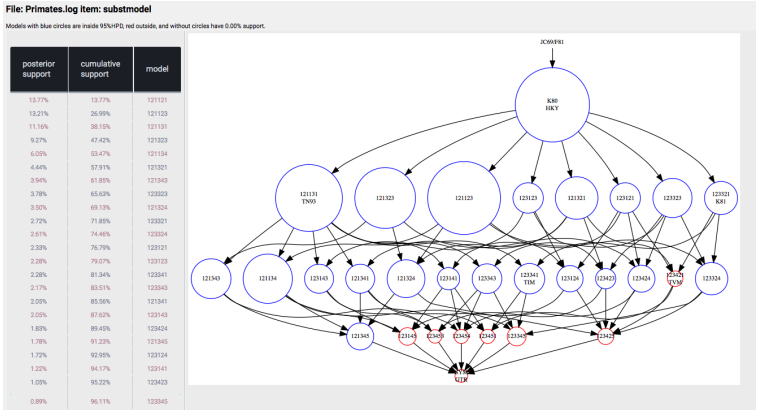
Model comparison of topologies

- Clade support for two alternative clades – M_1: clade A is present M_2: clade B is present
- From sample from prior: $P(M_1) = 0.3$ $P(M_2) = 0.4$
- From sample from posterior: $P(D|M_1) = 0.6$ $P(D|M_2) = 0.1$
- Bayes factor

$$\frac{p(D|M_1)}{p(D|M_2)} = \frac{\frac{posterior(M_1)}{prior(M_1)}}{\frac{posterior(M_2)}{prior(M_2)}} = \frac{\frac{0.6}{0.3}}{\frac{0.1}{0.4}} = 8$$

- Positive support for M_1 for clade A vs clade B

Model comparison of substitution models



- bModelTest – M_1: HKY vs M_2: GTR
- From sample from prior: $P(M_1) = \frac{1}{31}$ $P(M_2) = \frac{1}{31}$
- From sample from posterior: $P(D|M_1) = 0.1377$ $P(D|M_2) = 0.006$
- Bayes factor

$$\frac{p(D|M_1)}{p(D|M_2)} = \frac{\frac{posterior(M_1)}{prior(M_1)}}{\frac{posterior(M_2)}{prior(M_2)}} = \frac{0.1377/\frac{1}{31}}{0.006/\frac{1}{31}} = 22.95$$

- Strong support for M_1: HKY

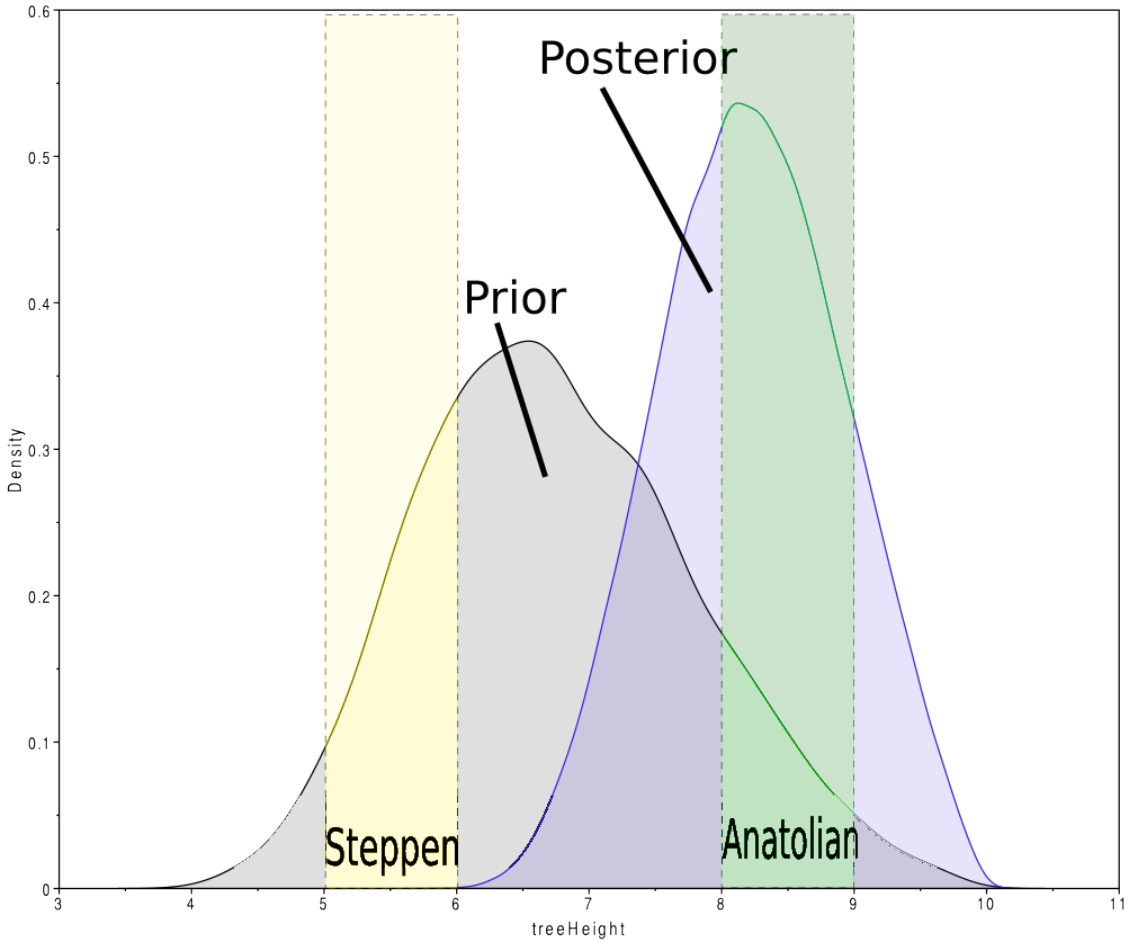
Model comparison of root age

Origin of Indo-European: Two competing theories

Steppen 5000 – 6000BP, Anatolian 8000 – 9000BP

Model comparison of root age

Origin of Indo-European: Two competing theories

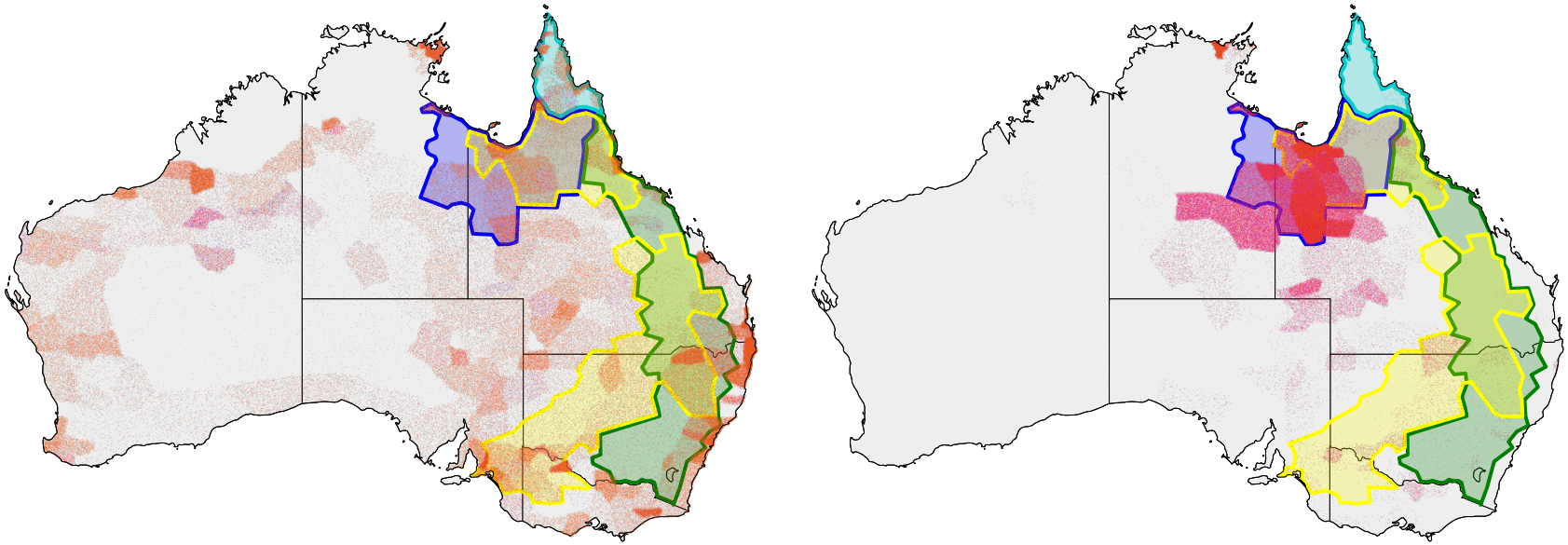


Root height Prior = 6.8 [4.9, 8.8] Posterior 8.2 [6.9, 9.6]

Bayes Factor $\gg$ 100 in favour of Anatolian hypothesis

Model comparison of root location

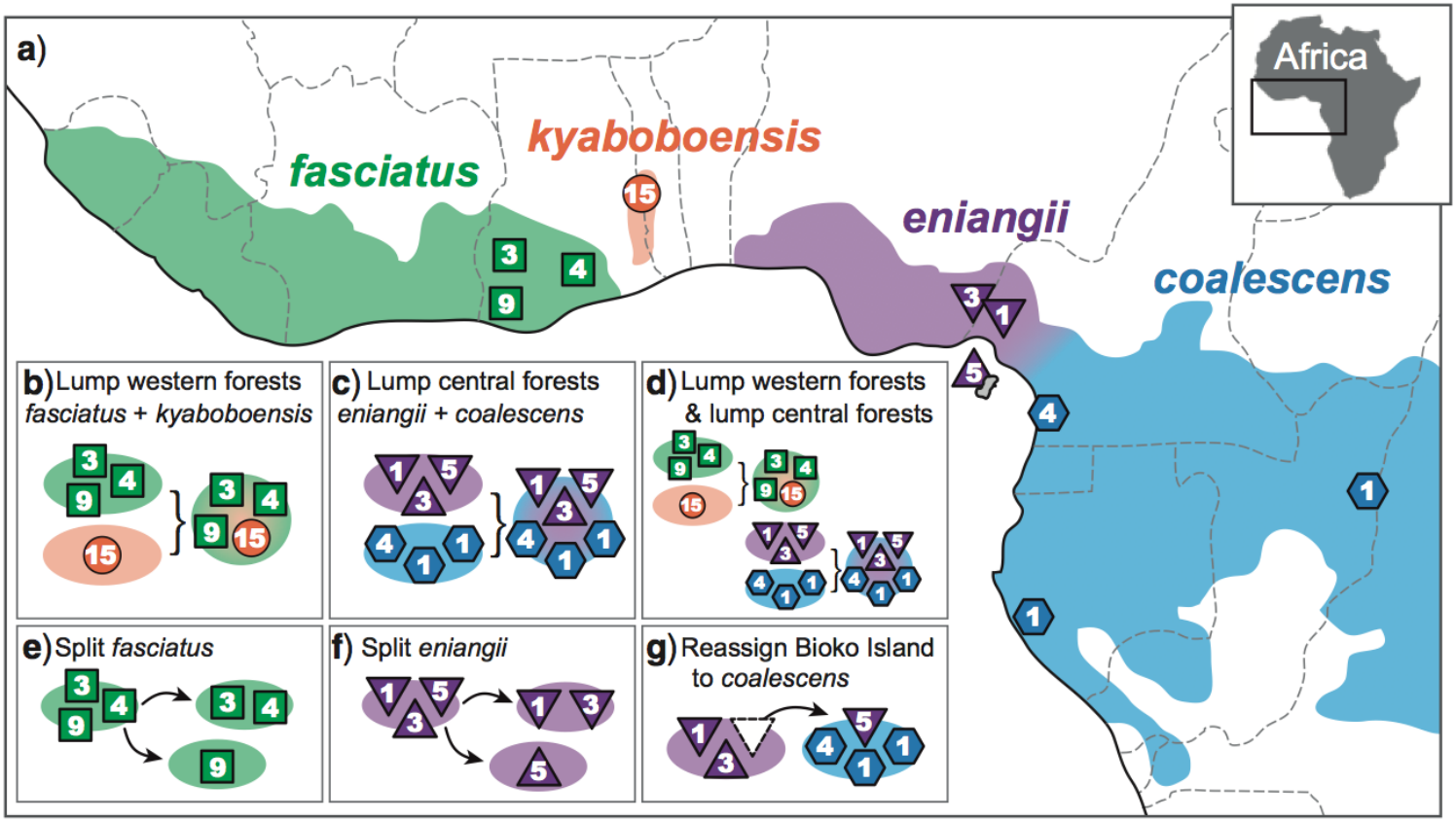
Root location: Pama Nyungang M_1 M_2 M_3 M_4



Bayes Factors:

	M_1	M_2	M_3	M_4
M_1	–	6.22	76.66	486.34
M_2	0.16	–	12.33	78.23
M_3	0.01	0.08	–	6.34
M_4	0.00	0.01	0.16	–

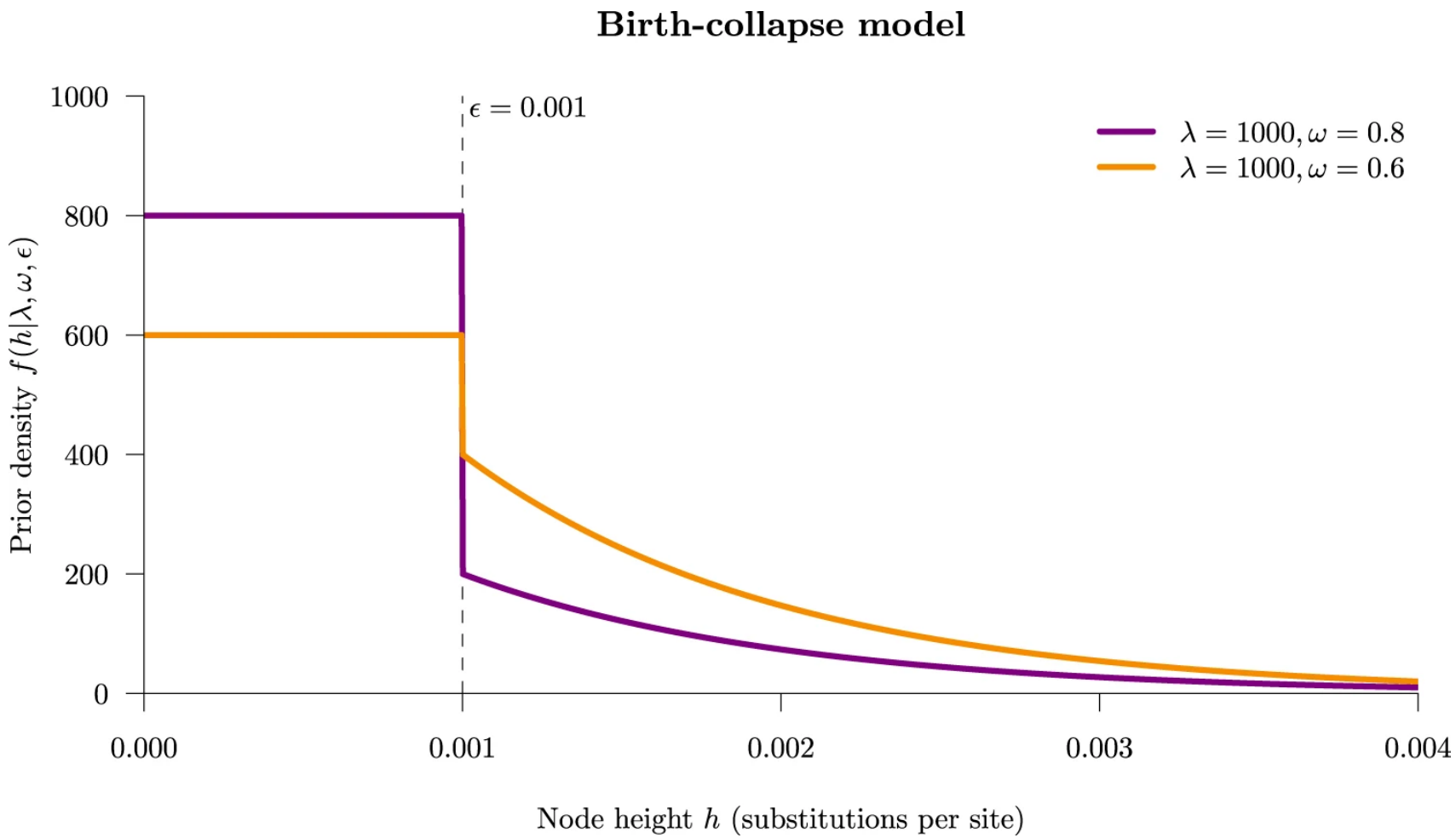
Species delimitation – BFD = Bayes Factor Delimitation



Model	#Species	ML	Rank	BF
a. Current taxonomy	4	−12890.3	2	–
b. Lump western forests	3	−15024.5	6	4268.3
c. Lump central forests	3	−14094.0	5	2407.4
d. Lump western & central forests	2	−16190.4	7	6600.3
e. Split fasciatus	5	−13088.0	3	395.5
f. Split eniangii	5	−12615.3	1	−550.0
g. Reassign Bioko Island	4	−13434.4	4	1088.2

Leache et al, 2014

Species delimitation – SpeeDemon

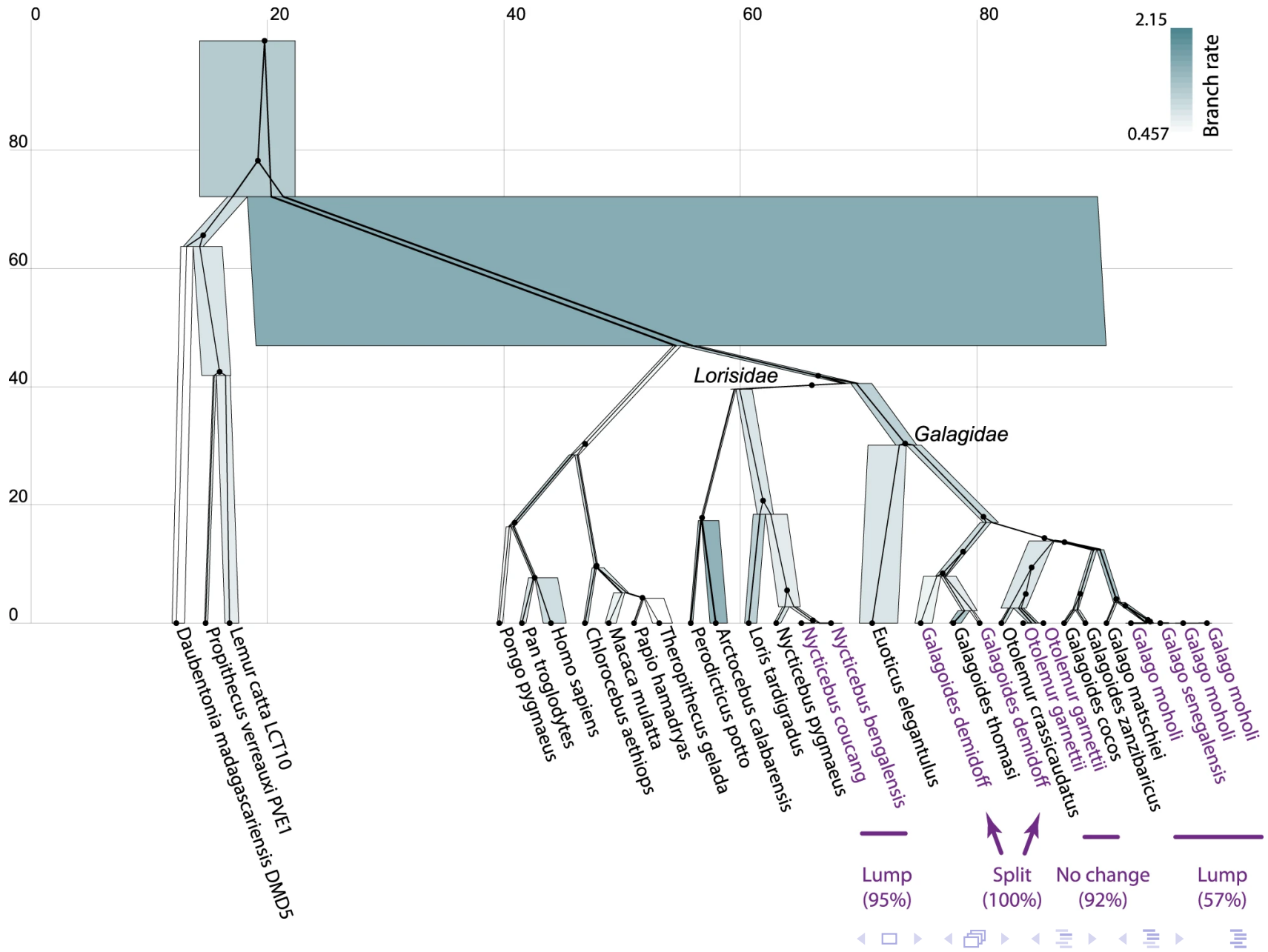


Tree prior: Yule skyline collapse

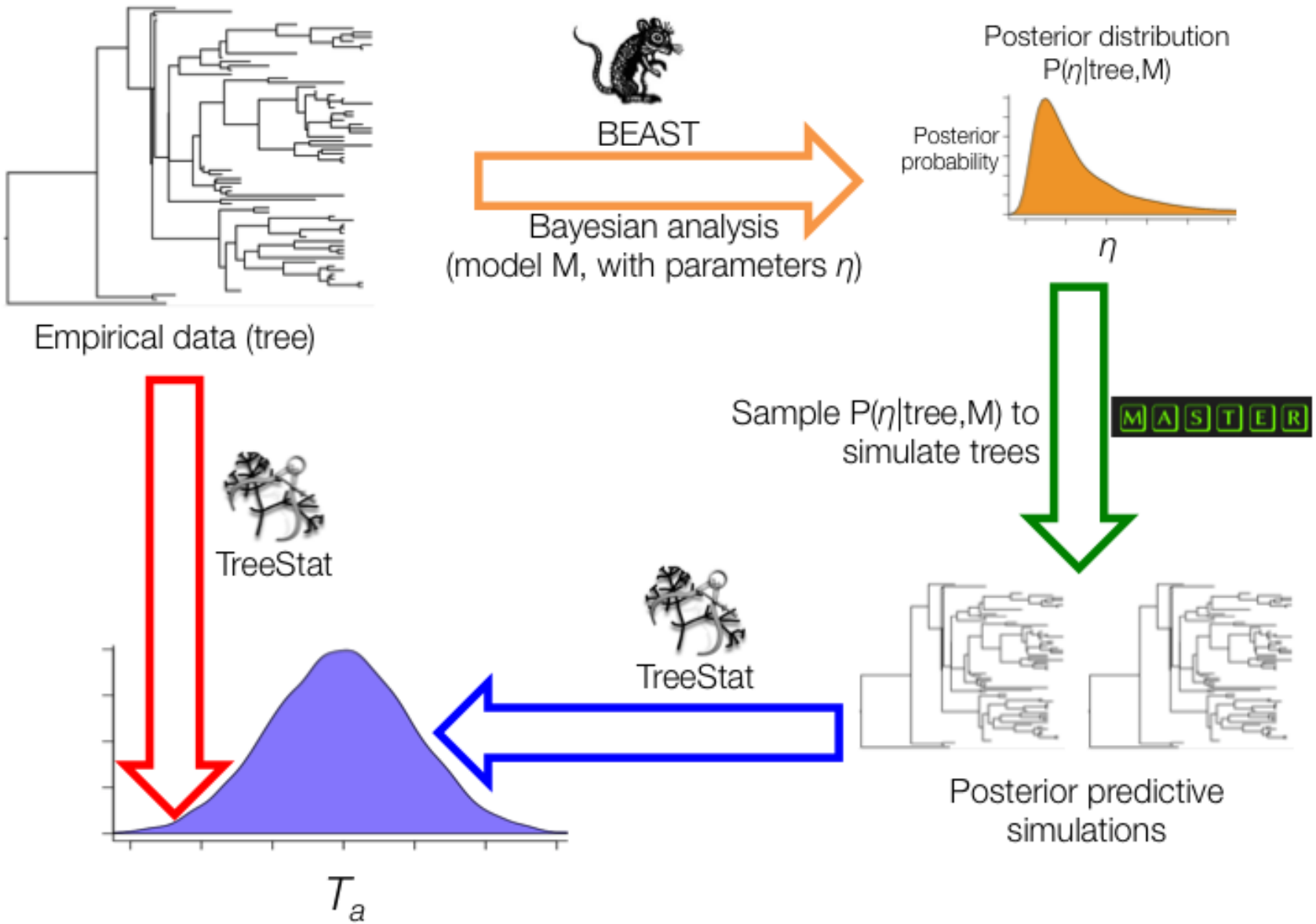
Douglas & Bouckaert, 2022

Species delimitation – SpeeDemon

Species delimitation – SpeeDemon



Model adequacy: Is this model adequate for my data?

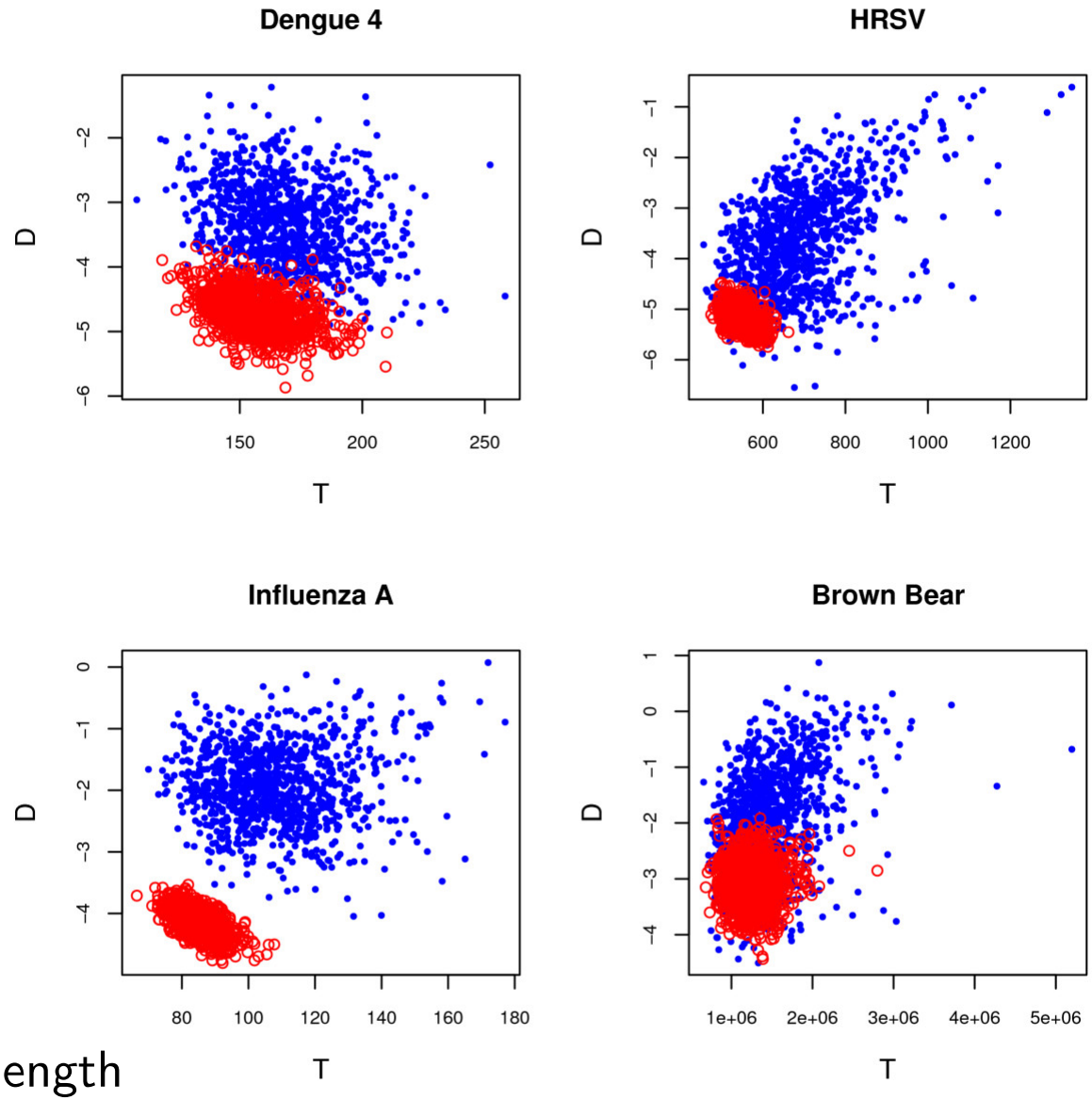


Model adequacy: Is this model adequate for my data?

Posterior predictive simulation:

- Sample from posterior
- Generate data for each posterior sample
- Calculate summary statistics on generated data and actual data
  - frequency of nucleotides (for different substitution models)
- Use loss function to compare statistics
  - Deviance loss function L: $\sum_{x \in \{A,C,G,T\}} log(\frac{\pi_x}{\hat{\pi}_x})$
  - Criterion $E\{L\} + L$
- Automates goldilocks zone:
  - If model is too simple, goodness of fit of mean statistic will be low
  - If model is too complex, variability of statistic will be high

Model adequacy: test of neutrality



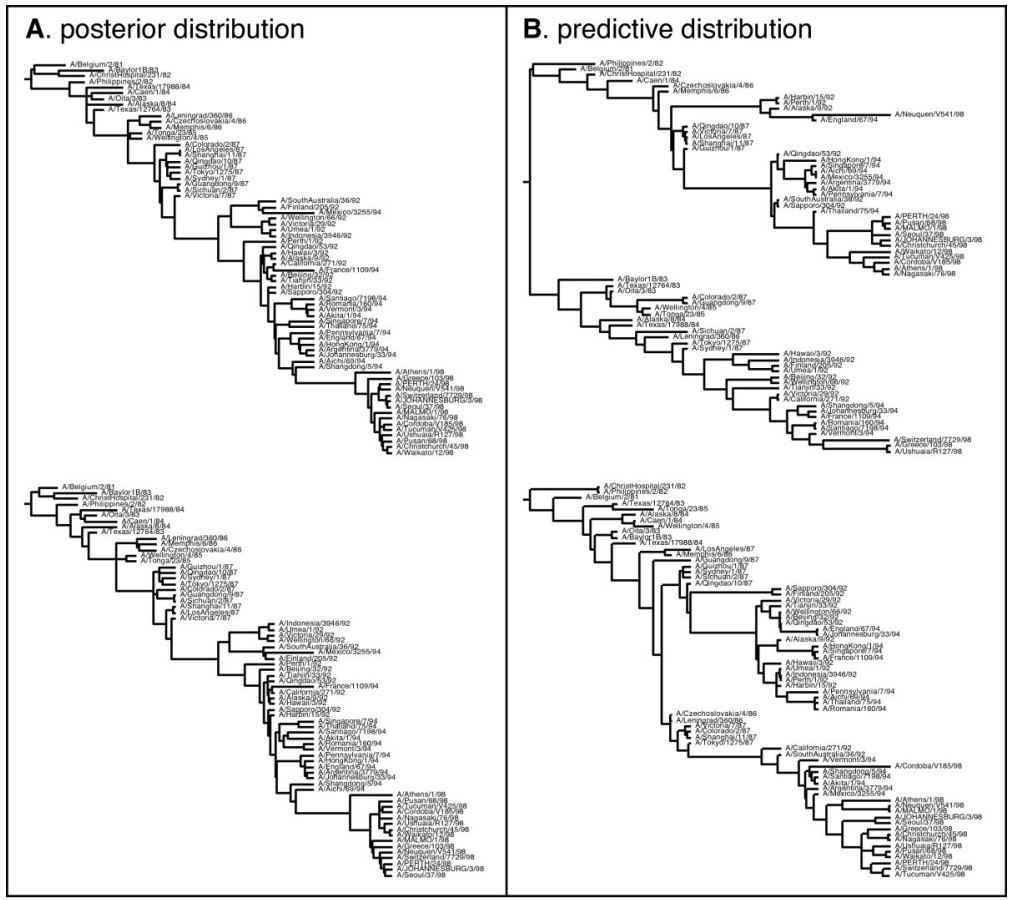
T = total tree length

D = Normalised difference between external branch lengths and total tree length.

Drummond & Suchard, BMC Genetics, 2008

Model adequacy: test of neutrality

Tree shape human influenza A virus



Note the shorter tree length and absence of deep splits in the posterior trees.

Drummond & Suchard, BMC Genetics, 2008

Summary model comparison, selection & averaging

Questions?

Thanks: Patricio Russell for slides