## simdata

POPULATION SIZE, MIGRATION, DIVERGENCE, ASSIGNMENT, HISTORY

Bayesian inference using the structured coalescent

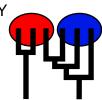
Migrate-n version 5.1.1(git:v5.0.2-50-gc469c7c) [March-31-2024]

Compiled for PARALLEL computer architectures

One master and 10 compute nodes are available.

Program started at Sun Mar 31 18:01:12 2024

Program finished at Sun Mar 31 18:02:48 2024 [Runtime:0000:00:01:36]



## **Options**

Inheritance multipliers in use for Thetas:

All loci use an inheritance multiplier of 1.0

Random number seed: (from parmfile) 427203015

Start parameters:

Theta values were generated Using a percent value of the prior

M values were generated Using a percent value of the prior

Connection matrix:

m = average (average over a group of Thetas or M,

s = symmetric migration M, S = symmetric 4Nm,

0 = zero, and not estimated,

\* = migration free to vary, Thetas are on diagonal

d = row population split off column population, D = split and then migration

Population 1 2 3
1 Romanshorn\_0 \* 0 0
2 Arbon\_1 d \* 0
3 Kreuzlingen\_2 0 d \*

Order of parameters:

1  $\Theta_1$  <displayed>

2	$\Theta_2$	<displayed></displayed>	
3	$\Theta_3^-$	<displayed></displayed>	
4	$\Delta^{\circ}_{1\rightarrow 2}$	<displayed></displayed>	
5	σ <sub>1-&gt;2</sub>	<displayed></displayed>	
6	$\Delta$ <sub>2-&gt;3</sub>	<displayed></displayed>	
7	σ <sub>2-&gt;3</sub>	<displayed></displayed>	

Mutation rate among loci:

Mutation rate is constant for all loci

Bayesian inference

Analysis strategy:

-Population size estimation: Exponential Distribution

-Geneflow estimation: Exponential Distribution

-Divergence time estimation: Normal Distribution (mean and standard dev.)

#### Proposal distributions for parameter

Parameter Proposal
Theta Metropolis sampling
M Metropolis sampling
Divergence Metropolis sampling
Divergence Spread Metropolis sampling
Genealogy Metropolis-Hastings

#### Prior distribution for parameter

Par	ameter		Prio	r Minimum	Mean*	Maximum	Delta	Bins	UpdateFreq
1	Theta	* *	Uniform	0.000000	0.050	0.100	0.010000	1500	0.07143
2	Theta	* *	Uniform	0.000000	0.050	0.100	0.010000	1500	0.07143
3	Theta	* *	Uniform	0.000000	0.050	0.100	0.010000	1500	0.07143
4	Splittime mean	1 2	Gamma	0.000000	0.100	0.800	(a=1.50)	1500	0.07143
5	Splittime std	1 2	Gamma	0.000000	0.100	0.200	(a=1.50)	1500	0.07143
6	Splittime mean	2 3	Uniform	0.000000	0.005	0.010	0.000100	1500	0.07143
7	Splittime std	2 3	Uniform	0.000000	0.005	0.010	0.000100	1500	0.07143

<sup>[\* \*</sup> means priors were set globally]

#### Posterior distribution:

Parameter values were collected using MCMC, these values were then used to generate the posterior histograms using BINNING and subsequent MOVING AVERAGE SMOOTHING (window=41) for combination over loci

Markov chain settings:

Number of chains

Long chain

1

Recorded steps [a]			1	0000
Increment (record every x step [b]				100
Number of concurrent chains (replicates) [c]				1
Visited (sampled) parameter values [a*b*c]			100	0000
Number of discard trees per chain (burn-in)				1000
Multiple Markov chains:				
Static heating scheme		4 chains	with tempe	ratures
	1000000.00	3.00	1.50	1.00
		Swa	apping inter	val is 1
Print options:				
Data file:				infile
			p	armfile
Haplotyping is turned on:				NO
Output file:				outfile
Posterior distribution raw histogram file:			ba	ayesfile
Raw data from the MCMC run:			bayesa	ıllfile.gz
Print data:				No
Print genealogies [only some for some data type]:				None

## Data summary

Data file:

Datatype:

Haplotype data

Number of loci:

Mutationmodel parameters

### Mutationmodel: Locus Sublocus

1	1	Jukes-Cantor	[Basefreq: =0.25]
2	1	Jukes-Cantor	[Basefreq: =0.25]
3	1	Jukes-Cantor	[Basefreq: =0.25]
4	1	Jukes-Cantor	[Basefreq: =0.25]
5	1	Jukes-Cantor	[Basefreq: =0.25]
6	1	Jukes-Cantor	[Basefreq: =0.25]
7	1	Jukes-Cantor	[Basefreq: =0.25]
8	1	Jukes-Cantor	[Basefreq: =0.25]
9	1	Jukes-Cantor	[Basefreq: =0.25]
10	1	Jukes-Cantor	[Basefreq: =0.25]

Mutationmodel

#### Sites per locus

Locus	Sites
1	500
2	500
3	500
4	500
5	500
6	500
7	500
8	500
9	500
10	500

Site rate variation and probabilities:

Locus Sublocus Region type Rate of change Probability Patch size

1	1	1	1.000	1.000	1.000
2	1	1	1.000	1.000	1.000
3	1	1	1.000	1.000	1.000
4	1	1	1.000	1.000	1.000
5	1	1	1.000	1.000	1.000
6	1	1	1.000	1.000	1.000

7	1 1	1.000	1.000	1.000		
	1 1	1.000	1.000	1.000		
	1 1	1.000	1.000	1.000		
	1 1	1.000	1.000	1.000		
Population				Locus	Gene c	opies
					data	(missing)
1 Romansh	norn_0			1	10	
				2	10	
				3	10	
				4	10	
				5	10	
				6	10	
				7	10	
				8	10	
				9	10	
				10	10	
2 Arbon_1				1	10	
				2	10	
				3	10	
				4	10	
				5	10	
				6	10	
				7	10	
				8	10	
				9	10	
				10	10	
3 Kreuzling	jen_2			1	10	
				2	10	
				3	10	
				4	10	
				5	10	
				6 7	10 10	
				8	10	
				9	10	
				10	10	
Total of all	populations			10	30	(0)
i otal of all	populations			2	30	(0)
				3	30	(0)
				4	30	(0)
				5	30	(0)
				6	30	(0)
				7	30	(0)
				8	30	(0)
				9	30	(0)
						. ,

10	30	(0)
.0	00	(0)

# Bayesian Analysis: Posterior distribution table

Locus	Parameter	2.5%	25.0%	Mode	75.0%	97.5%	Median	Mean
1	$\Theta_1$	0.00447	0.00940	0.01317	0.01813	0.03387	0.01577	0.01742
1	$\Theta_2$	0.00147	0.00507	0.00757	0.01053	0.01927	0.00883	0.00961
1	$\Theta_3^2$	0.00000	0.00353	0.00610	0.00940	0.02093	0.00783	0.00912
1	D <sub>1-&gt;2</sub>	0.00107	0.07040	0.11973	0.14613	0.19680	0.10480	0.10287
1	S <sub>1-&gt;2</sub>	0.00240	0.01520	0.04767	0.07853	0.17160	0.07007	0.07780
1	D <sub>2-&gt;3</sub>	0.00009	0.00136	0.00334	0.00482	0.00897	0.00394	0.00433
1	S <sub>2-&gt;3</sub>	0.00027	0.00033	0.00081	0.00206	0.00657	0.00472	0.00485
2	$\Theta_1$	0.00553	0.01053	0.01483	0.01993	0.03680	0.01757	0.01936
2	$\Theta_2$	0.00000	0.00180	0.00337	0.00500	0.00873	0.00390	0.00396
2	$\Theta_3$	0.00173	0.00560	0.00863	0.01253	0.02580	0.01077	0.01212
2	D <sub>1-&gt;2</sub>	0.00053	0.06560	0.11440	0.14240	0.19520	0.10160	0.10051
2	S <sub>1-&gt;2</sub>	0.00413	0.01760	0.05447	0.08187	0.17187	0.07180	0.07912
2	D <sub>2-&gt;3</sub>	0.00066	0.00284	0.00491	0.00695	0.00980	0.00509	0.00511
2	S <sub>2-&gt;3</sub>	0.00151	0.00717	0.00786	0.00899	0.00993	0.00573	0.00572
3	$\Theta_1$	0.00733	0.01333	0.01910	0.02520	0.04687	0.02223	0.02444
3	$\Theta_2$	0.00000	0.00213	0.00377	0.00560	0.00993	0.00443	0.00459
3	$\Theta_3$	0.00000	0.00293	0.00530	0.00833	0.02000	0.00697	0.00834
3	D <sub>1-&gt;2</sub>	0.00000	0.05333	0.09520	0.12213	0.17867	0.08880	0.08961
3	S <sub>1-&gt;2</sub>	0.00200	0.01600	0.04140	0.07667	0.16920	0.06767	0.07575
3	$D_{2->3}$	0.00009	0.00149	0.00322	0.00499	0.00813	0.00394	0.00431
3	S <sub>2-&gt;3</sub>	0.00067	0.00082	0.00114	0.00193	0.00978	0.00506	0.00512
4	$\Theta_1$	0.00153	0.00527	0.00790	0.01133	0.02140	0.00957	0.01047
4	$\Theta_2$	0.00073	0.00400	0.00617	0.00873	0.01527	0.00710	0.00758
4	$\Theta_3$	0.00207	0.00680	0.01077	0.01593	0.03733	0.01383	0.01637
4	D <sub>1-&gt;2</sub>	0.00213	0.07573	0.12133	0.15307	0.20107	0.10853	0.10619
4	S <sub>1-&gt;2</sub>	0.00280	0.01907	0.04540	0.08280	0.17173	0.07100	0.07844
4	D <sub>2-&gt;3</sub>	0.00061	0.00247	0.00484	0.00660	0.00967	0.00483	0.00490
4	S <sub>2-&gt;3</sub>	0.00161	0.00599	0.00634	0.00669	0.00994	0.00594	0.00586
5	$\Theta_1$	0.00507	0.01087	0.01497	0.02060	0.03820	0.01790	0.01960
5	$\Theta_2$	0.00093	0.00427	0.00657	0.00933	0.01713	0.00770	0.00839
5	$\Theta_3$	0.00000	0.00173	0.00337	0.00513	0.00993	0.00417	0.00431
5	D <sub>1-&gt;2</sub>	0.00000	0.05760	0.10053	0.12640	0.18080	0.09200	0.09175

Migrate 5.1.1(git:v5.0.2-50-gc469c7c): (http://popgen.sc.fsu.edu) [program run on 18:01:12]

_ocus	Parameter	2.5%	25.0%	Mode	75.0%	97.5%	Median	Mean
5	S <sub>1-&gt;2</sub>	0.00213	0.01507	0.04073	0.07653	0.16840	0.06753	0.07566
5	D <sub>2-&gt;3</sub>	0.00056	0.00215	0.00383	0.00603	0.00970	0.00464	0.00484
5	S <sub>2-&gt;3</sub>	0.00032	0.00044	0.00091	0.00421	0.00942	0.00485	0.00493
6	$\Theta_1$	0.00567	0.01080	0.01423	0.02053	0.03833	0.01803	0.01986
6	$\Theta_{2}$	0.00067	0.00400	0.00630	0.00893	0.01680	0.00743	0.00808
6	$\Theta_3$	0.00000	0.00147	0.00297	0.00460	0.00887	0.00363	0.00368
6	D <sub>1-&gt;2</sub>	0.00267	0.08693	0.15280	0.17920	0.22720	0.12400	0.12100
6	S <sub>1-&gt;2</sub>	0.00440	0.02600	0.04420	0.08080	0.17733	0.07833	0.08453
6	D <sub>2-&gt;3</sub>	0.00123	0.00363	0.00486	0.00758	0.00990	0.00545	0.00541
6	S <sub>2-&gt;3</sub>	0.00034	0.00066	0.00318	0.00371	0.00877	0.00476	0.00487
7	$\Theta_1$	0.00600	0.01127	0.01517	0.02087	0.03787	0.01837	0.02009
7	$\Theta_2$	0.00447	0.00907	0.01250	0.01687	0.02987	0.01463	0.01584
7	$\Theta_3$	0.00007	0.00293	0.00503	0.00740	0.01413	0.00610	0.00661
7	D <sub>1-&gt;2</sub>	0.00053	0.06613	0.11067	0.13600	0.18773	0.09840	0.09719
7	S <sub>1-&gt;2</sub>	0.00227	0.01373	0.03767	0.07480	0.16960	0.06673	0.07545
7	D <sub>2-&gt;3</sub>	0.00090	0.00297	0.00481	0.00694	0.00982	0.00510	0.00512
7	S <sub>2-&gt;3</sub>	0.00054	0.00273	0.00312	0.00463	0.00969	0.00490	0.00498
8	$\Theta_1$	0.00567	0.01107	0.01503	0.02093	0.03813	0.01830	0.02005
8	$\Theta_2$	0.00087	0.00400	0.00610	0.00847	0.01493	0.00697	0.00740
8	$\Theta_3$	0.00127	0.00547	0.00837	0.01227	0.02533	0.01043	0.01179
8	D <sub>1-&gt;2</sub>	0.00267	0.07253	0.12240	0.14827	0.19840	0.10587	0.10414
8	S <sub>1-&gt;2</sub>	0.00280	0.01653	0.03420	0.08200	0.17067	0.07220	0.07963
8	D <sub>2-&gt;3</sub>	0.00165	0.00421	0.00522	0.00760	0.00985	0.00538	0.00531
8	S <sub>2-&gt;3</sub>	0.00240	0.00713	0.00868	0.00965	0.00995	0.00635	0.00628
9	$\Theta_1$	0.00920	0.01673	0.02257	0.03053	0.05473	0.02683	0.02928
9	$\Theta_2$	0.00000	0.00273	0.00450	0.00647	0.01127	0.00517	0.00546
9	$\Theta_3$	0.00267	0.00793	0.01217	0.01880	0.04540	0.01650	0.01968
9	D <sub>1-&gt;2</sub>	0.00000	0.06080	0.10480	0.13387	0.18827	0.09627	0.09615
9	S <sub>1-&gt;2</sub>	0.00320	0.01800	0.04647	0.08013	0.17093	0.06913	0.07717
9	D <sub>2-&gt;3</sub>	0.00008	0.00173	0.00360	0.00523	0.00907	0.00408	0.00435
9	S <sub>2-&gt;3</sub>	0.00127	0.00414	0.00526	0.00747	0.00989	0.00552	0.00553
10	$\Theta_1$	0.01067	0.01800	0.02430	0.03260	0.05833	0.02877	0.03136
10	$\Theta_2$	0.00593	0.01113	0.01510	0.02007	0.03480	0.01750	0.01887
10	$\Theta_3^-$	0.00107	0.00500	0.00783	0.01207	0.02767	0.01037	0.01231
10	D <sub>1-&gt;2</sub>	0.00160	0.07360	0.12560	0.15360	0.20373	0.10800	0.10612
10	S <sub>1-&gt;2</sub>	0.00293	0.01653	0.03420	0.08067	0.16573	0.07073	0.07852

Migrate 5.1.1(git:v5.0.2-50-gc469c7c): (http://popgen.sc.fsu.edu) [program run on 18:01:12]

Locus	Parameter	2.5%	25.0%	Mode	75.0%	97.5%	Median	Mean
10 10	D <sub>2-&gt;3</sub> S <sub>2-&gt;3</sub>	0.00094 0.00018	0.00313 0.00026	0.00490 0.00069	0.00666 0.00314	0.00986 0.00904	0.00511 0.00421	0.00521 0.00452
All	$\Theta_1$	0.01160	0.01427	0.01590	0.01760	0.02113	0.01623	0.01628
All All	$\Theta_2$ $\Theta_3$	0.00367	0.00547 0.00527	0.00663 0.00650	0.00773	0.00967 0.00973	0.00670 0.00657	0.00668 0.00654
AII AII AII	D <sub>1-&gt;2</sub> S <sub>1-&gt;2</sub> D <sub>2-&gt;3</sub>	0.09600 0.01587 0.00232	0.11840 0.04960 0.00347	0.13040 0.06820 0.00375	0.14187 0.08600 0.00468	0.16320 0.14253 0.00629	0.13093 0.07273 0.00418	0.13017 0.07576 0.00424
All	S <sub>2-&gt;3</sub>	0.00251	0.00321	0.00457	0.00541	0.00964	0.00576	0.00582

#### Citation suggestions:

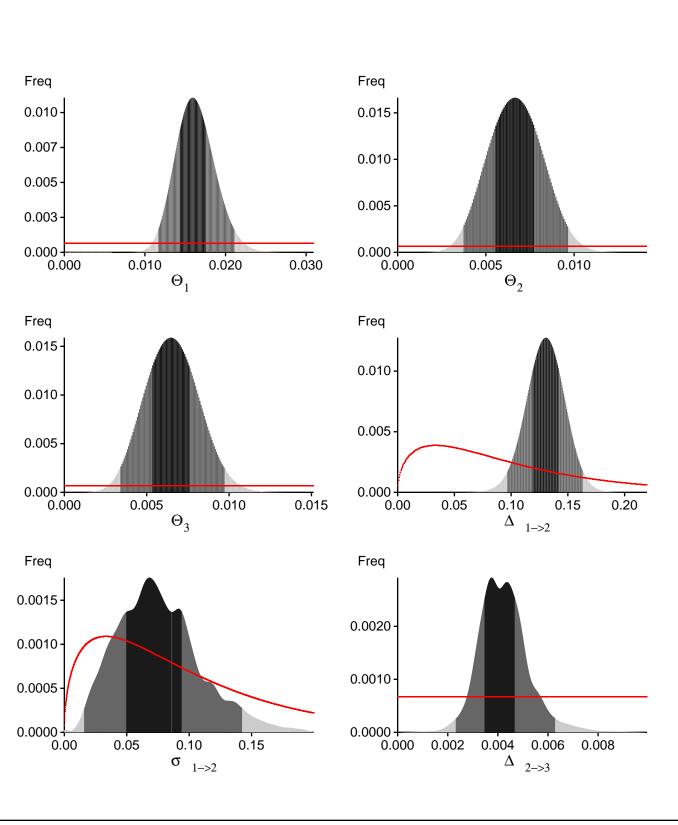
Beerli P., 2006. Comparison of Bayesian and maximum-likelihood inference of population genetic parameters. Bioinformatics 22:341-345

Beerli, P., H. Ashki, S. Mashayekhi, and M. Palczewski, 2022. Population divergence time estimation using individual lineage label switching. G3 Genesâ Genomesâ Genetics, 12(4), 02 2022.

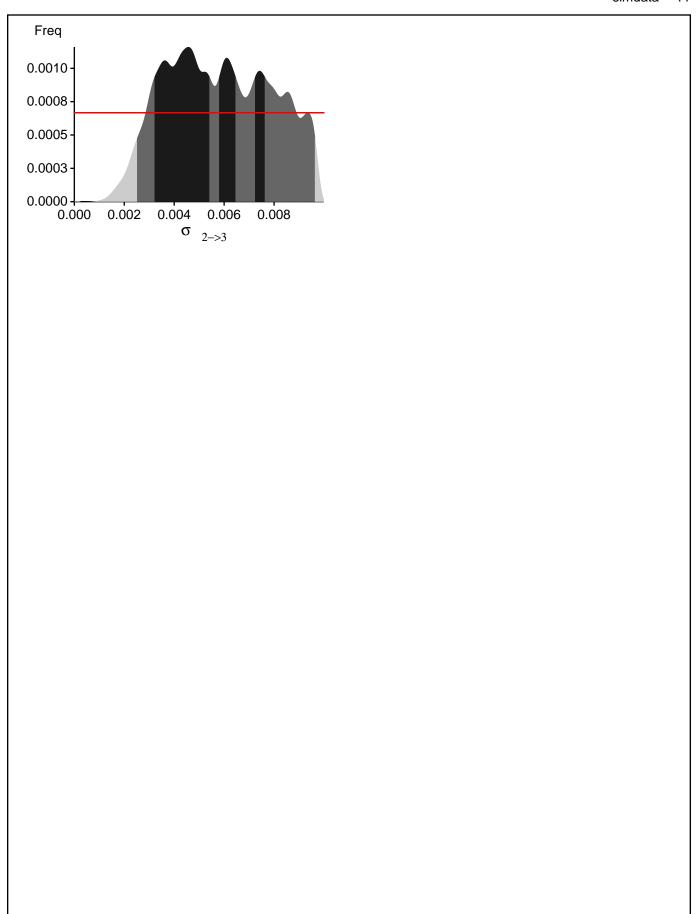
Beerli P., 2009. How to use MIGRATE or why are Markov chain Monte Carlo programs difficult to use? In Population Genetics for Animal Conservation, G. Bertorelle, M. W. Bruford, H. C. Hauffe, A. Rizzoli, and C. Vernesi, eds., vol. 17 of Conservation Biology, Cambridge University Press, Cambridge UK, pp. 42-79.

Beerli, P., S. Mashayekhi, M. Sadeghi, M. Khodaei, and K. Shaw, 2019. Population genetic inference with migrate Current Protocols in Bioinformatics, 68(1):e87.

## Bayesian Analysis: Posterior distribution over all loci



Migrate 5.1.1(git:v5.0.2-50-gc469c7c): (http://popgen.sc.fsu.edu) [program run on 18:01:12]



Migrate 5.1.1(git:v5.0.2-50-gc469c7c): (http://popgen.sc.fsu.edu) [program run on 18:01:12]

## Log-Probability of the data given the model (marginal likelihood)

Use this value for Bayes factor calculations:

BF = Exp[ In(Prob(D | thisModel) - In( Prob( D | otherModel) or as LBF = 2 (In(Prob(D | thisModel) - In( Prob( D | otherModel)) shows the support for thisModel]

Locus	TI(1a)	BTI(1b)	HS(3)	
1	-1585.76	-1453.94	-1435.89	
2	-1637.74	-1459.90	-1434.32	
3	-1503.82	-1389.95	-1370.74	
4	-1549.64	-1414.31	-1396.20	
5	-1511.06	-1386.76	-1371.15	
6	-1638.30	-1474.70	-1452.92	
7	-1766.69	-1549.36	-1516.53	
8	-1702.31	-1527.14	-1500.76	
9	-1686.84	-1520.97	-1497.88	
10	-2031.14	-1741.16	-1695.38	
All	-16632.63	-14937.51	-14691.10	

- (1a) TI: Thermodynamic integration: log(Prob(D|Model)): Good approximation with many temperatures
- (1b) BTI: Bezier-approximated Thermodynamic integration: when using few temperatures USE THIS!
- (2) SS: Steppingstone Sampling (Xie et al 2011)
- (3) HS: Harmonic mean approximation: Overestimates the marginal likelihood, poor variance [Scaling factor = -19.323628]

Citation suggestions:

Beerli P. and M. Palczewski, 2010. Unified framework to evaluate panmixia and migration direction among multiple sampling locations, Genetics, 185: 313-326.

Palczewski M. and P. Beerli, 2014. Population model comparison using multi-locus datasets.

In M.-H. Chen, L. Kuo, and P. O. Lewis, editors, Bayesian Phylogenetics: Methods, Algorithms, and Applications, pages 187-200. CRC Press, 2014.

Xie W., P. O. Lewis, Y. Fan, L. Kuo, and M.-H. Chen. 2011. Improving marginal likelihood estimation for Bayesian phylogenetic model selection. Systematic Biology, 60(2):150â 160, 2011.

# Acceptance ratios for all parameters and the genealogies

Parameter	Accepted changes	Ratio
$\Theta_1$	329347/714044	0.46124
$\Theta_2$	349350/714176	0.48917
$\Theta_3$	345162/714990	0.48275
$\Delta_{1\rightarrow 2}$	474578/714180	0.66451
$\sigma_{1\rightarrow 2}$	488259/713891	0.68394
$\Delta$ 2->3	556584/713444	0.78014
σ 2->3	544684/715739	0.76101
Genealogies	1162109/4999536	0.23244

# MCMC-Autocorrelation and Effective MCMC Sample Size

Parameter	Autocorrelation	Effective Sampe Size
$\Theta_1$	0.40940	42797.20
$\Theta_2$	0.50608	33653.94
$\Theta_3^2$	0.52572	32793.44
$\Delta_{1\rightarrow 2}$	0.05596	89434.58
$\sigma_{1\rightarrow 2}$	0.08476	84408.27
$\Delta$ $2\rightarrow 3$	0.17867	69781.22
$\sigma_{2\rightarrow 3}$	0.23977	61731.56
Genealogies	0.40940	42797.20

# Average temperatures during the run

# Chain Temperatures 1 0.00000 2 0.00000 3 0.00000 4 0.00000

Adaptive heating often fails, if the average temperatures are very close together try to rerun using static heating! If you want to compare models using marginal likelihoods then you MUST use static heating

## Potential Problems

This section reports potential problems with your run, but such reporting is often not very accurate. With many parameters in a multilocus analysis, it is common that some parameters for some loci will not be informative. These parameters then trigger suggestions to increase the prior range that are not sensible. Do not blindly follow the suggestions given. If some parameters are flagged, inspect the tables carefully and judge whether an action is required. Suppose you run a Bayesian inference with sequence data for macroscopic species. In that case, there is rarely the need to increase the prior for Theta beyond 0.1. If you use microsatellites data, it is rather common that your prior distribution for Theta should have a range from 0.0 to 100 or more. With many populations (>3), it is also very common that some migration routes are estimated poorly because the data contains little or no information for that route. Increasing the prior range will not help in such situations, but reducing the number of parameters may help.

Param 13 (Locus 8): Upper prior boundary seems too low!