

# Aggregated sampling output

November 20, 2020

**Dataset: experimental\_data\_d2eGFP, model type: ODE**

## Trajectories without pathologies

e.g. no divergent transitions, no max\_tredepth exceeded, no Rhat > 1.1, no n\_eff < 100

number of trajectories without pathologies (out of 100):

[1] 49

indices of trajectories without pathologies:

```
[1] 1 2 3 6 7 8 10 12 14 15 18 20 21 25 26 28 29 30 31
[20] 37 39 40 41 43 44 45 46 47 52 53 55 57 58 61 62 65 66 68
[39] 72 73 77 80 81 82 89 95 96 98 100
```

## no pathologies for a subset of the parameters

parameters considered:

```
[1] "t0" "sigma" "scale"
[4] "offset" "prod_theta2_m0_scale"
```

number of trajectories without pathologies (out of 100):

[1] 59

indices of trajectories without pathologies:

```
[1] 1 2 3 6 7 8 9 10 11 12 14 15 18 20 21 25 26 27 28
[20] 29 30 31 33 37 39 40 41 43 44 45 46 47 52 53 55 57 58 61
[39] 62 63 64 65 66 68 69 71 72 73 77 80 81 82 83 84 89 95 96
[58] 98 100
```

## Divergent transitions

num..of.div..transitions	Freq
0	92
1	6
2	2

total number of trajectories with div. transitions: 8

indices of trajectories with div. transitions:

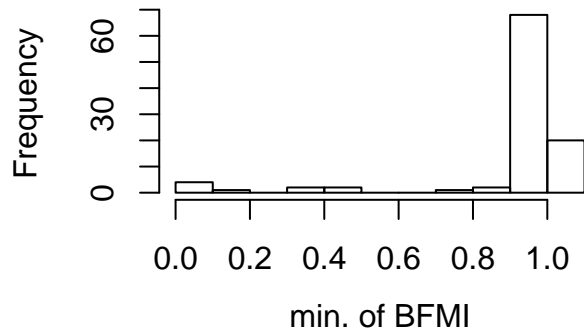
19 22 38 59 78 79 85 93

## Maximum tree depth exceeded

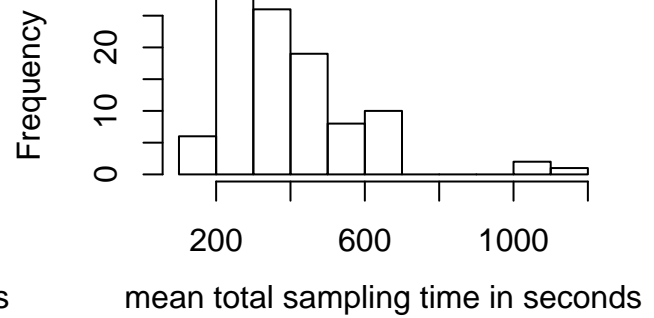
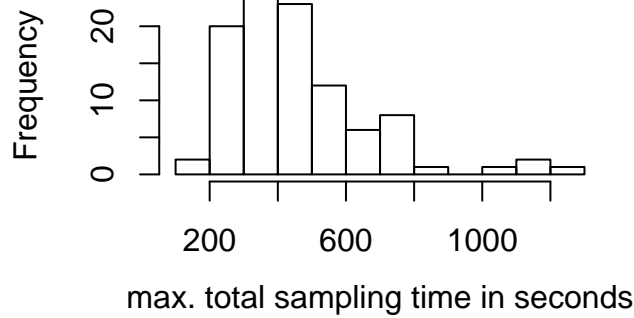
num..of.max.t.d..exceeded	Freq
0	100

### Bayesian fraction of missing information (BFMI)

num..of.low.BFMI	Freq
0	95
1	2
2	3



### Total sampling time



### R-hat

total number of trajectories with very high Rhat ( $> 1.1$ ) (out of 100)

[1] 44

number of trajectories with high Rhat per parameter (out of 100)

	Rhat $> 1.02$	Rhat $> 1.1$
theta[1]	14	9
theta[2]	0	0
theta[3]	13	9
m0	0	0
sigma	25	14
scale	0	0
offset	35	33
t0	36	35
prod_theta2_m0	0	0
prod_theta2_scale	0	0

	Rhat > 1.02	Rhat > 1.1
prod_m0_scale	0	0
prod_theta2_m0_scale	34	33
x2_sim[180]	0	0

number of parameters with high Rhat per trajectory (out of 13)

	4	5	9	11	13	16	17	22	23	24	27	32	33	34	35	36	42	48	49	50
Rhat > 1.02	3	3	2	2	4	4	4	4	4	4	3	3	2	4	4	4	3	4	4	3
Rhat > 1.1	3	3	2	2	4	3	3	4	4	3	2	3	2	3	4	3	1	3	4	3

	51	54	56	57	60	63	64	67	69	70	71	74	75	76	79	83	84	86	87	88
Rhat > 1.02	4	6	4	2	3	2	2	4	2	3	2	4	4	2	4	2	2	4	3	5
Rhat > 1.1	4	3	3	0	3	2	2	4	0	3	2	4	4	1	3	2	2	4	3	3

theta[1]

number of trajectories with Rhat > 1.02: 14

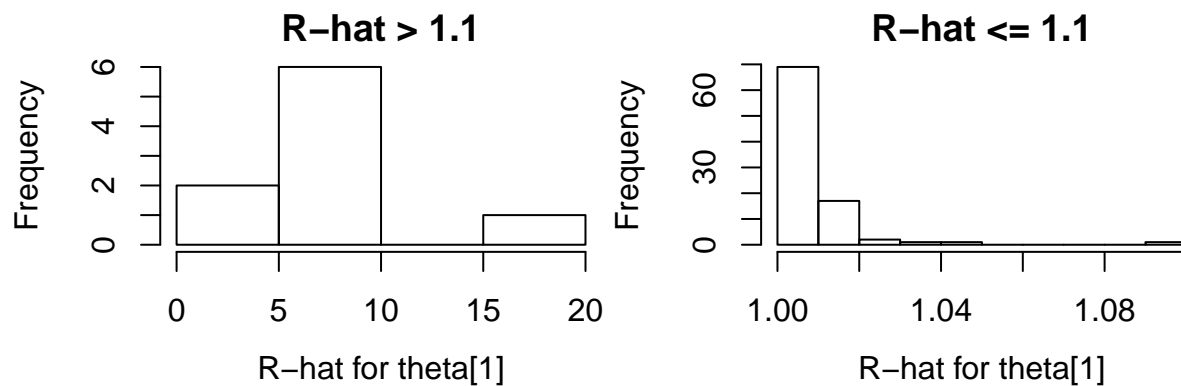
indices of trajectories with Rhat > 1.02:

9 11 27 33 54 57 63 64 69 71 83 84 88 90

number of trajectories with Rhat > 1.1: 9

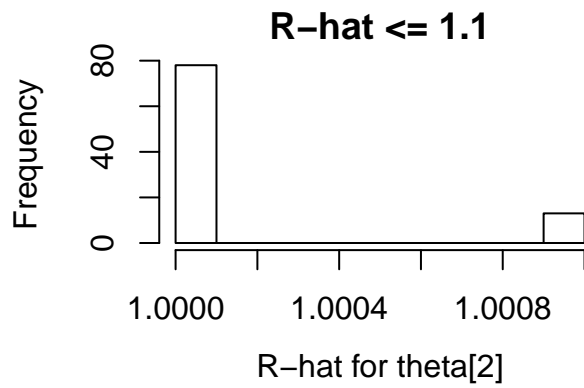
indices of trajectories with Rhat > 1.1:

9 11 27 33 63 64 71 83 84



theta[2]

no Rhat > 1.02



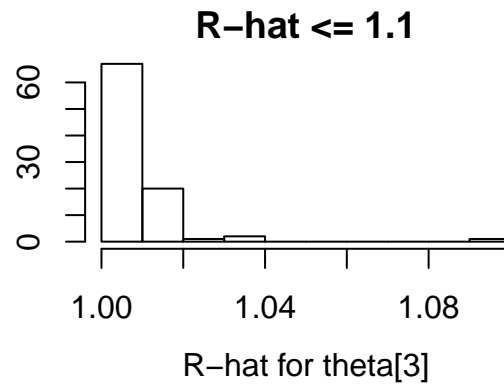
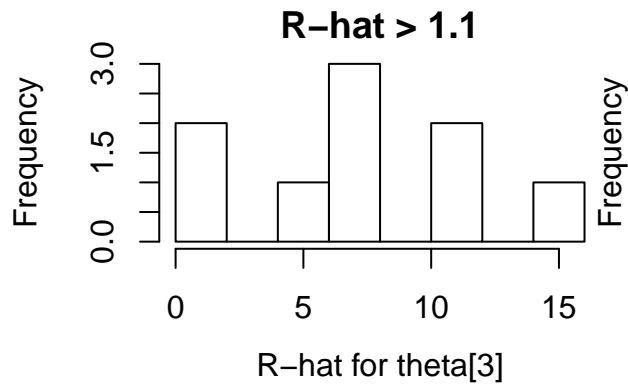
**theta[3]**

number of trajectories with Rhat > 1.02: 13

indices of trajectories with Rhat > 1.02:  
9 11 27 33 54 57 63 64 69 71 83 84 90

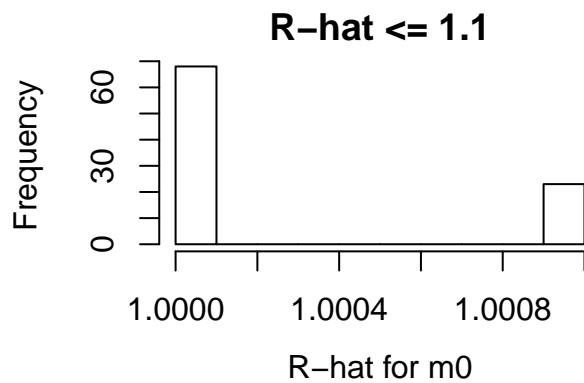
number of trajectories with Rhat > 1.1: 9

indices of trajectories with Rhat > 1.1:  
9 11 27 33 63 64 71 83 84



**m0**

no Rhat > 1.02



## sigma

number of trajectories with  $R_{\text{hat}} > 1.02$ : 25

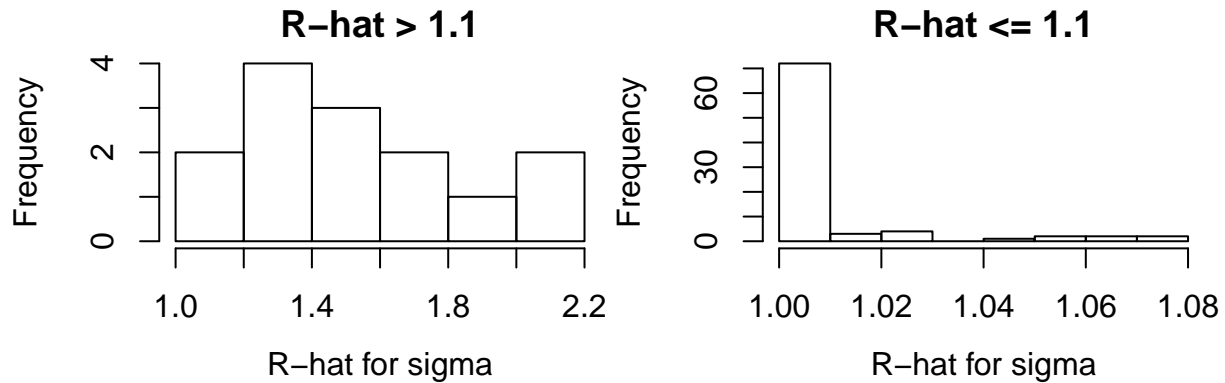
indices of trajectories with  $R_{\text{hat}} > 1.02$ :

13 16 17 22 23 24 34 35 36 48 49 51 54 56 67 74 75 79 86 88 91 92 94 97 99

number of trajectories with  $R_{\text{hat}} > 1.1$ : 14

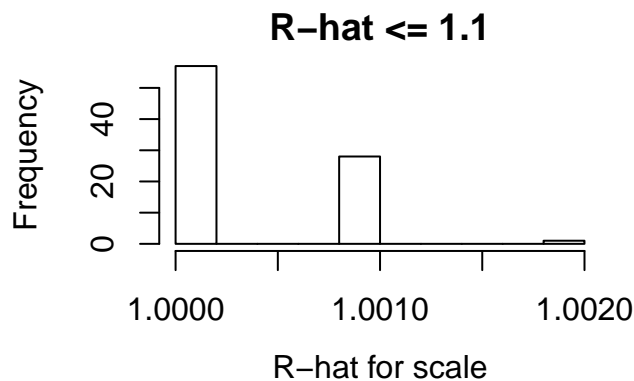
indices of trajectories with  $R_{\text{hat}} > 1.1$ :

13 22 23 35 49 51 67 74 75 86 91 94 97 99



## scale

no  $R_{\text{hat}} > 1.02$



## offset

number of trajectories with  $R_{\text{hat}} > 1.02$ : 35

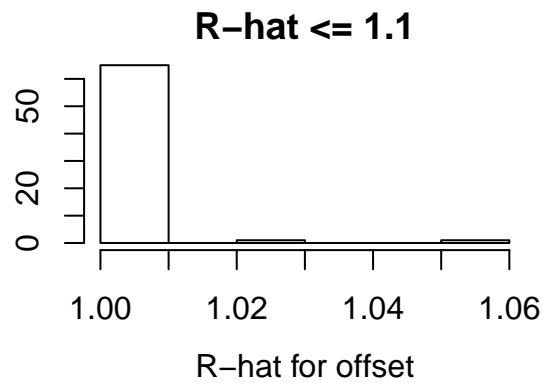
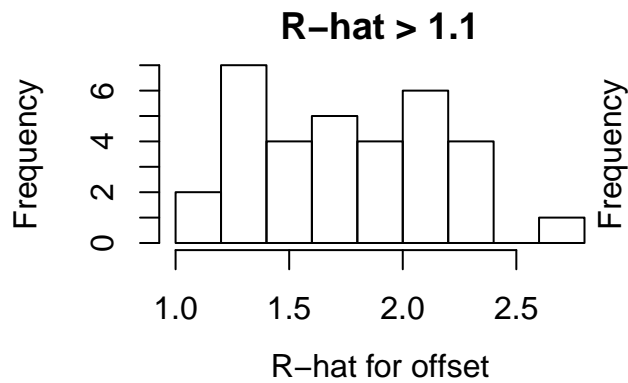
indices of trajectories with  $R_{\text{hat}} > 1.02$ :

4 5 13 16 17 22 23 24 32 34 35 36 42 48 49 50 51 54 56 60 67 70 74 75 76 79 86 87 88 90 91 92 94 97 99

number of trajectories with  $R_{\text{hat}} > 1.1$ : 33

indices of trajectories with  $R_{\text{hat}} > 1.1$ :

4 5 13 16 17 22 23 24 32 34 35 36 48 49 50 51 54 56 60 67 70 74 75 79 86 87 88 90 91 92 94 97 99



t0

number of trajectories with Rhat > 1.02: 36

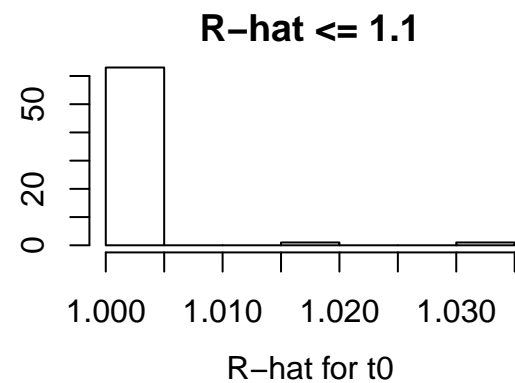
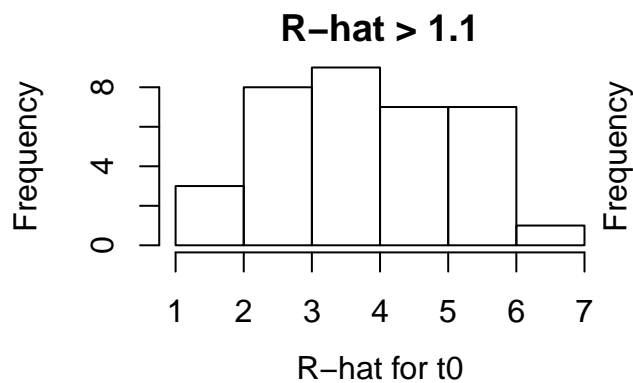
indices of trajectories with Rhat > 1.02:

4 5 13 16 17 22 23 24 27 32 34 35 36 42 48 49 50 51 54 56 60 67 70 74 75 76 79 86 87 88 90 91 92 94 97 99

number of trajectories with Rhat > 1.1: 35

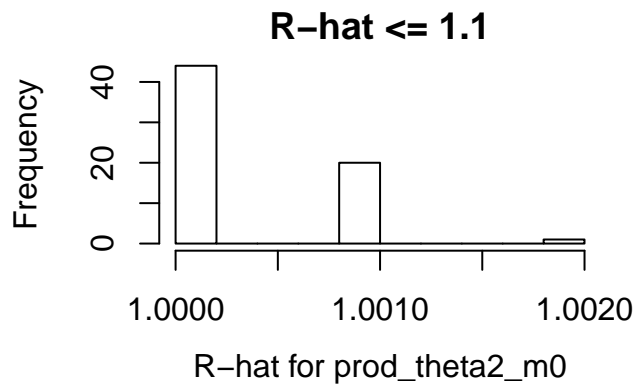
indices of trajectories with Rhat > 1.1:

4 5 13 16 17 22 23 24 32 34 35 36 42 48 49 50 51 54 56 60 67 70 74 75 76 79 86 87 88 90 91 92 94 97 99



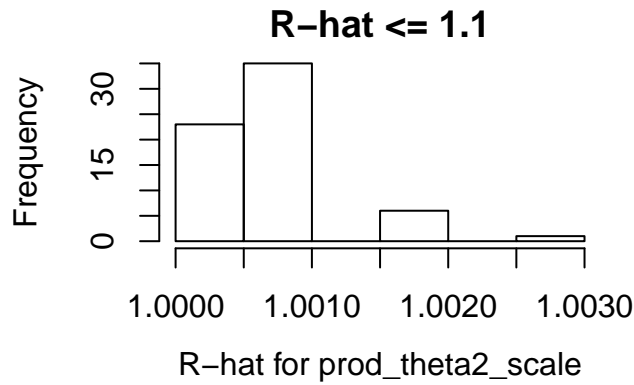
prod\_theta2\_m0

no Rhat > 1.02



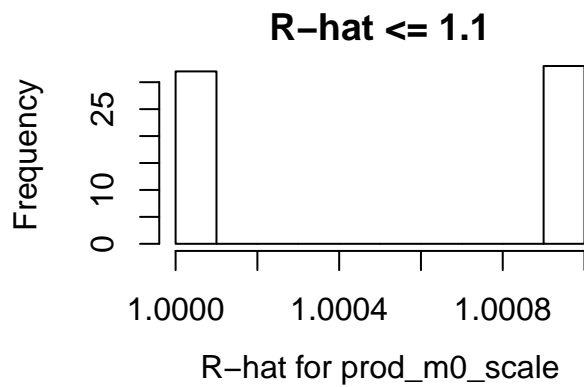
prod\_theta2\_scale

no Rhat > 1.02



prod\_m0\_scale

no Rhat > 1.02



prod\_theta2\_m0\_scale

number of trajectories with Rhat > 1.02: 34

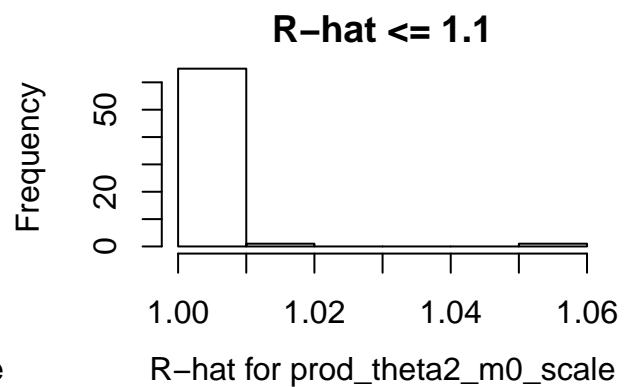
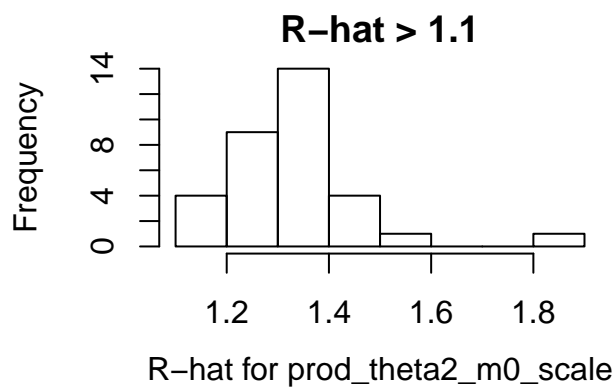
indizes of trajectories with Rhat > 1.02:

4 5 13 16 17 22 23 24 32 34 35 36 42 48 49 50 51 54 56 60 67 70 74 75 79 86 87 88 90 91 92 94 97 99

number of trajectories with Rhat > 1.1: 33

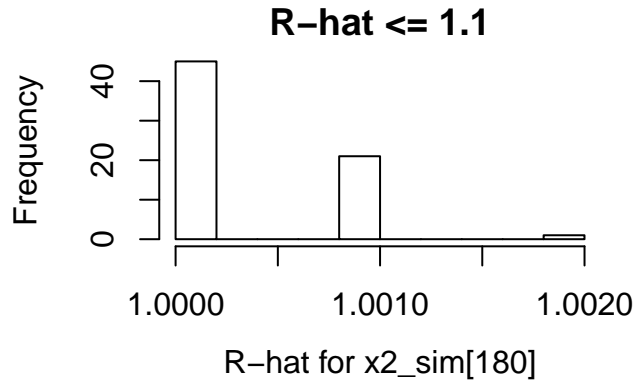
indices of trajectories with Rhat > 1.1:

4 5 13 16 17 22 23 24 32 34 35 36 48 49 50 51 54 56 60 67 70 74 75 79 86 87 88 90 91 92 94 97 99



x2\_sim[180]

no Rhat > 1.02



### Effective sample size (ESS)

total number of trajectories with low ESS (< 100) (out of 100)

[1] 45

number of trajectories with low ESS (< 100) per parameter (out of 100)

	n_eff < 100
theta[1]	10
theta[2]	0
theta[3]	10
m0	0
sigma	21
scale	0
offset	33
t0	35
prod_theta2_m0	0
prod_theta2_scale	0
prod_m0_scale	0
prod_theta2_m0_scale	33
x2_sim[180]	0

number of parameters with low ESS (< 300) per trajectory (out of 13)

	4	5	9	11	13	16	17	22	23	24	27	32	33	34	35	36	42	48	49	50
n_eff < 100	3	3	2	2	4	3	3	4	4	3	2	3	2	4	4	4	1	4	4	3

	51	54	56	60	63	64	67	69	70	71	74	75	76	79	83	84	86	87	88	90
n_eff < 100	4	4	4	3	2	2	4	2	3	2	4	4	1	4	2	2	4	3	4	3

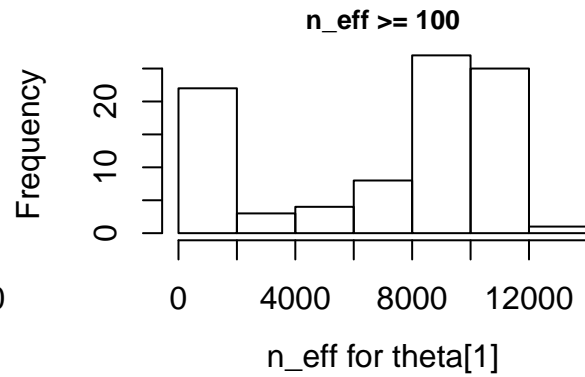
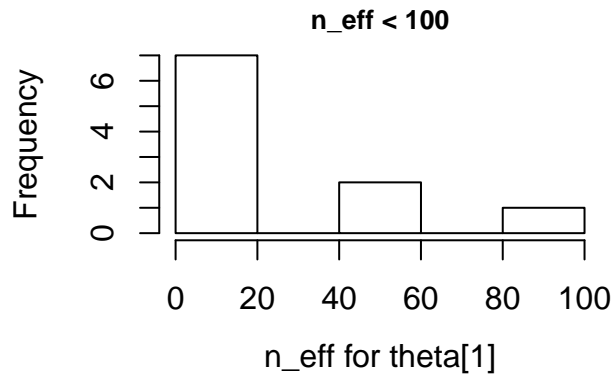
theta[1]

number of trajectories with n\_eff < 100: 10

indices of trajectories with n\_eff < 100:

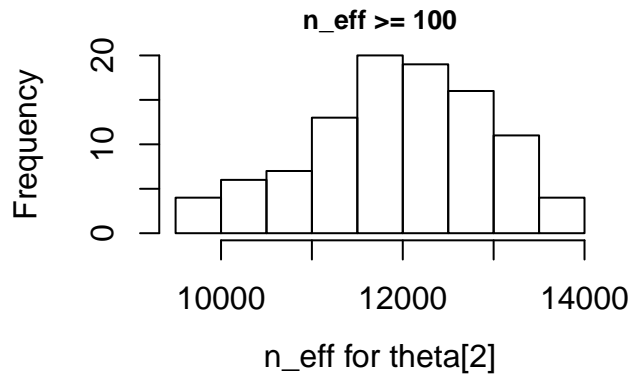


9 11 27 33 63 64 69 71 83 84



theta[2]

no n\_eff < 100

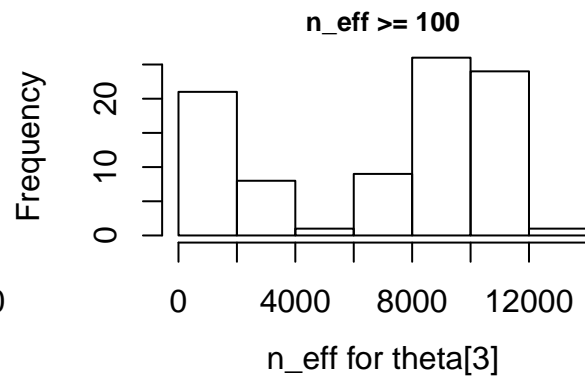
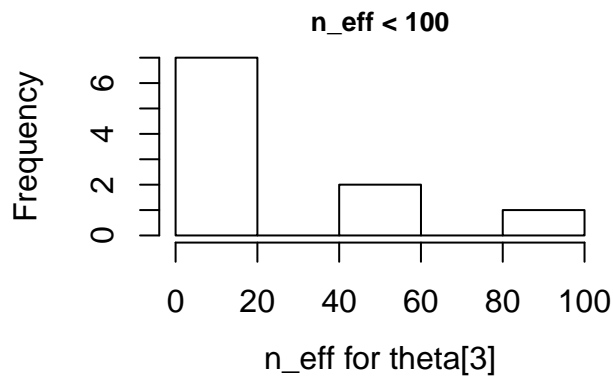


theta[3]

number of trajectories with n\_eff < 100: 10

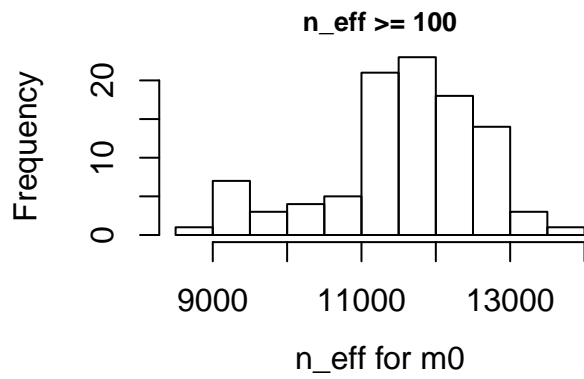
indices of trajectories with n\_eff < 100:

9 11 27 33 63 64 69 71 83 84



m0

no n\_eff < 100

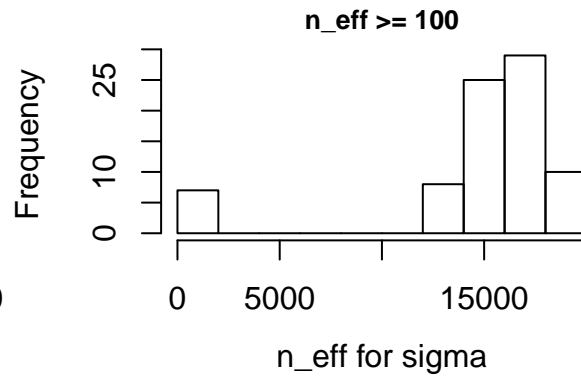
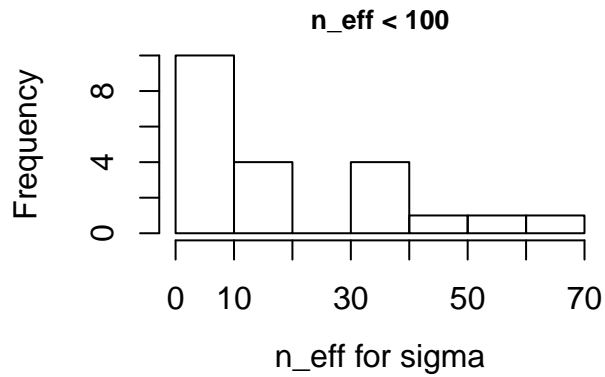


**sigma**

number of trajectories with n\_eff < 100: 21

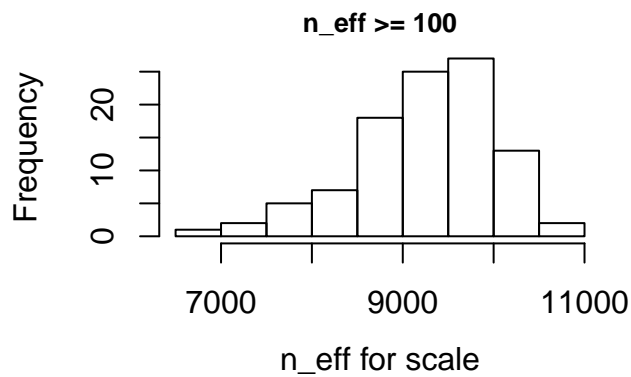
indices of trajectories with n\_eff < 100:

13 22 23 34 35 36 48 49 51 54 56 67 74 75 79 86 88 91 94 97 99



**scale**

no n\_eff < 100

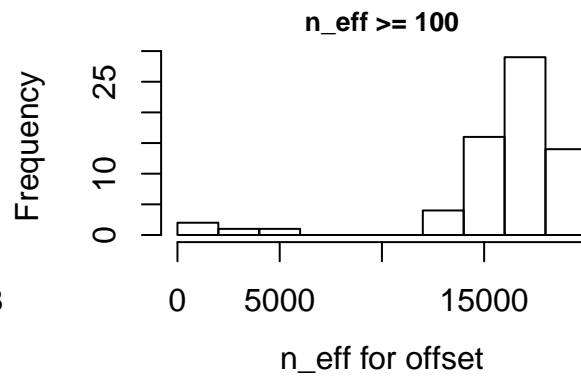
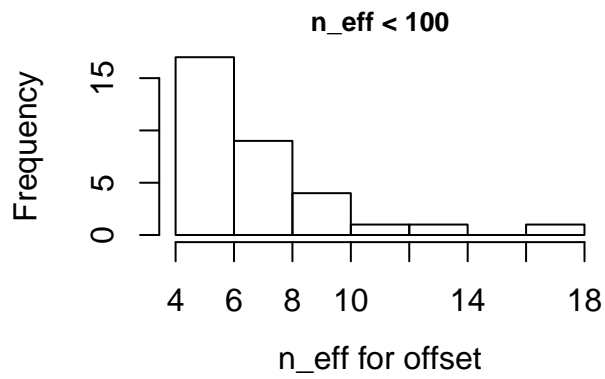


**offset**

number of trajectories with n\_eff < 100: 33

indices of trajectories with n\_eff < 100:

4 5 13 16 17 22 23 24 32 34 35 36 48 49 50 51 54 56 60 67 70 74 75 79 86 87 88 90 91 92 94 97 99

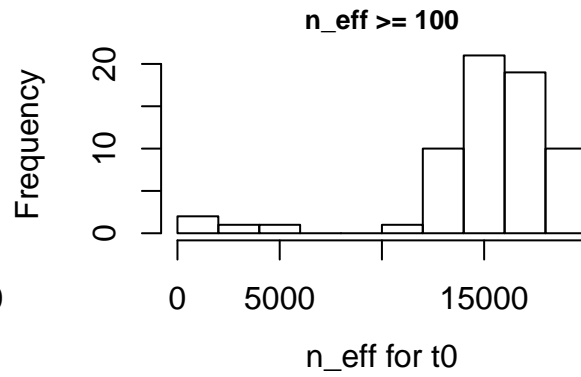
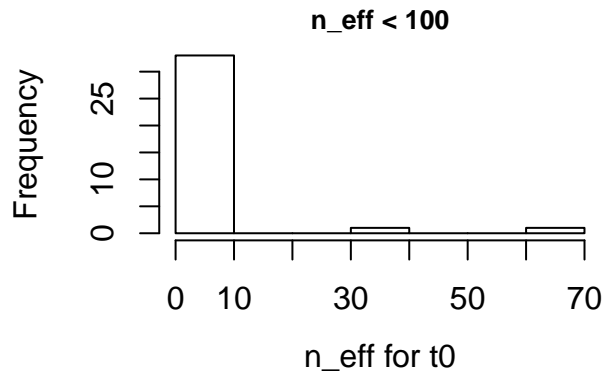


t0

number of trajectories with n\_eff < 100: 35

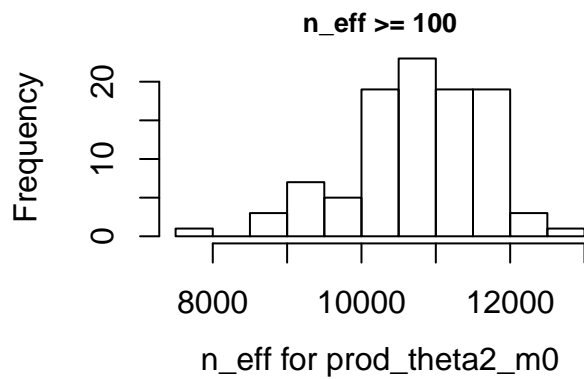
indices of trajectories with n\_eff < 100:

4 5 13 16 17 22 23 24 32 34 35 36 42 48 49 50 51 54 56 60 67 70 74 75 76 79 86 87 88 90 91 92 94 97 99



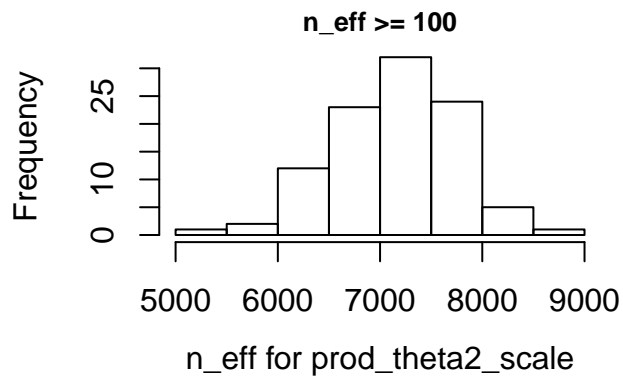
prod\_theta2\_m0

no n\_eff < 100



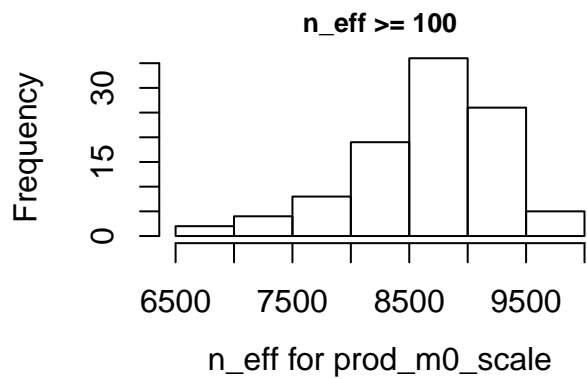
prod\_theta2\_scale

no n\_eff < 100



prod\_m0\_scale

no n\_eff < 100

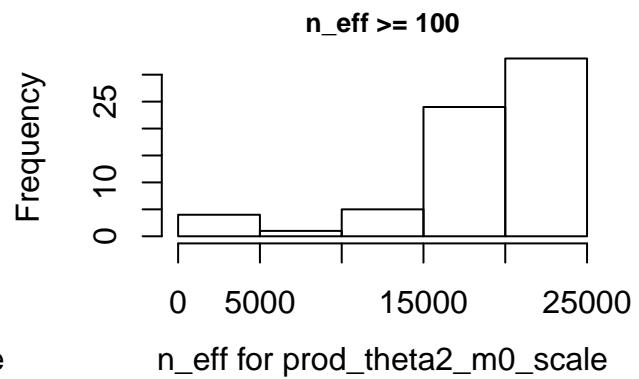
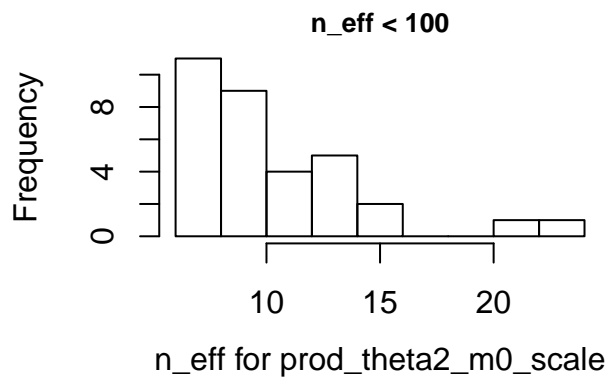


prod\_theta2\_m0\_scale

number of trajectories with n\_eff < 100: 33

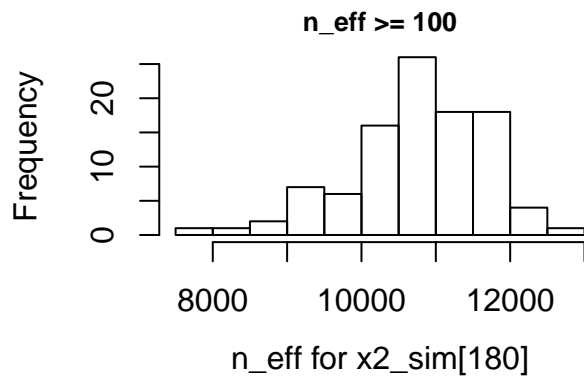
indices of trajectories with n\_eff < 100:

4 5 13 16 17 22 23 24 32 34 35 36 48 49 50 51 54 56 60 67 70 74 75 79 86 87 88 90 91 92 94 97 99



x2\_sim[180]

no n\_eff < 100



Find problematic trajectories and parameters

Are there any trajectories and parameters for which `n_eff` is below the threshold, but `Rhat` does not exceed the threshold?

```
## [1] FALSE
```

parameters per trajectories with very high `Rhat`

```
4:  offset  t0  prod_theta2_m0_scale
5:  offset  t0  prod_theta2_m0_scale
9:  theta[1] theta[3]
11: theta[1] theta[3]
13: sigma  offset  t0  prod_theta2_m0_scale
16: offset  t0  prod_theta2_m0_scale
17: offset  t0  prod_theta2_m0_scale
22: sigma  offset  t0  prod_theta2_m0_scale
23: sigma  offset  t0  prod_theta2_m0_scale
24: offset  t0  prod_theta2_m0_scale
27: theta[1] theta[3]
32: offset  t0  prod_theta2_m0_scale
33: theta[1] theta[3]
34: offset  t0  prod_theta2_m0_scale
35: sigma  offset  t0  prod_theta2_m0_scale
36: offset  t0  prod_theta2_m0_scale
42: t0
48: offset  t0  prod_theta2_m0_scale
49: sigma  offset  t0  prod_theta2_m0_scale
50: offset  t0  prod_theta2_m0_scale
51: sigma  offset  t0  prod_theta2_m0_scale
54: offset  t0  prod_theta2_m0_scale
56: offset  t0  prod_theta2_m0_scale
60: offset  t0  prod_theta2_m0_scale
63: theta[1] theta[3]
64: theta[1] theta[3]
67: sigma  offset  t0  prod_theta2_m0_scale
70: offset  t0  prod_theta2_m0_scale
71: theta[1] theta[3]
74: sigma  offset  t0  prod_theta2_m0_scale
75: sigma  offset  t0  prod_theta2_m0_scale
76: t0
79: offset  t0  prod_theta2_m0_scale
83: theta[1] theta[3]
84: theta[1] theta[3]
86: sigma  offset  t0  prod_theta2_m0_scale
```

```

87:  offset  t0  prod_theta2_m0_scale
88:  offset  t0  prod_theta2_m0_scale
90:  offset  t0  prod_theta2_m0_scale
91:  sigma  offset  t0  prod_theta2_m0_scale
92:  offset  t0  prod_theta2_m0_scale
94:  sigma  offset  t0  prod_theta2_m0_scale
97:  sigma  offset  t0  prod_theta2_m0_scale
99:  sigma  offset  t0  prod_theta2_m0_scale

```

### unique combinations:

number of unique combinations: 4

combinations and number of their occurrence:

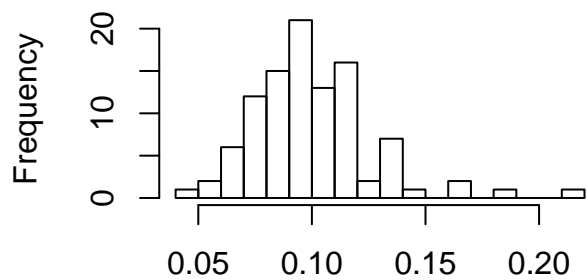
```

19 : offset  t0  prod_theta2_m0_scale
9  : theta[1]  theta[3]
14 : sigma  offset  t0  prod_theta2_m0_scale
2  : t0

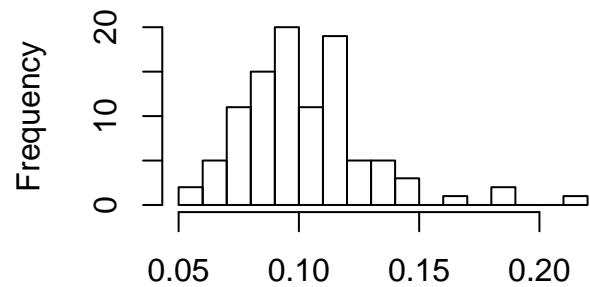
```

### Overview of estimates

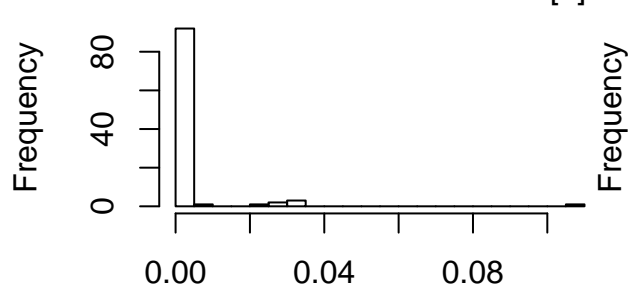
theta[1]



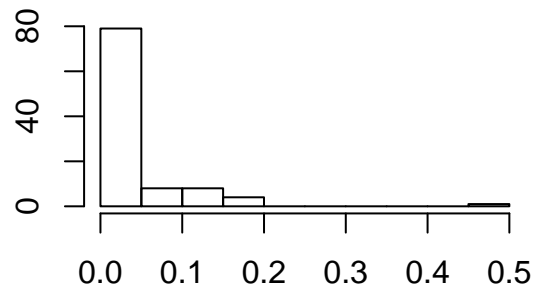
Median estimates for theta[1]



Mean estimates for theta[1]

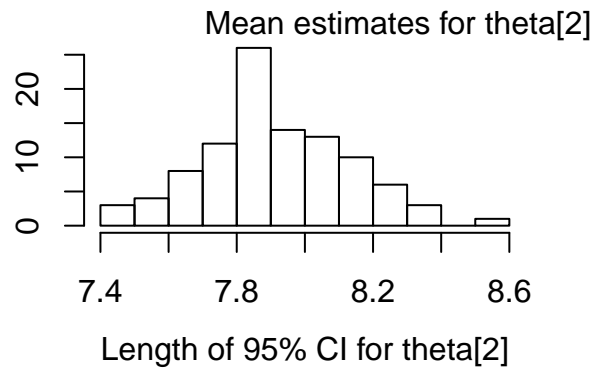
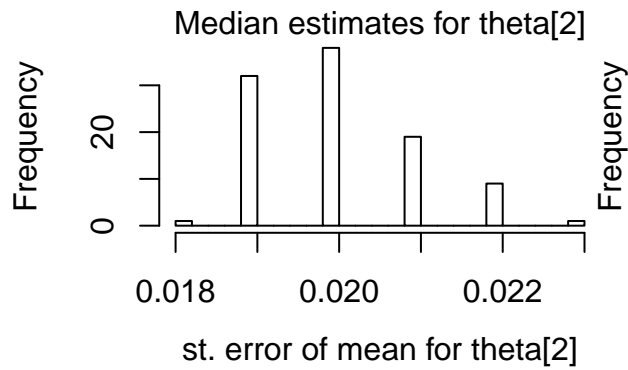
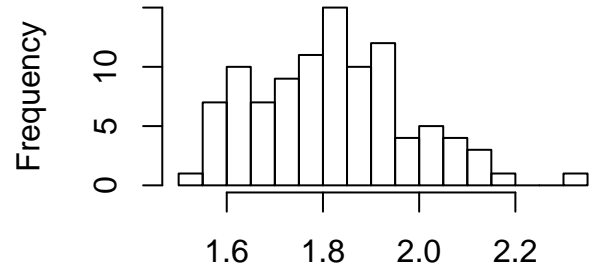
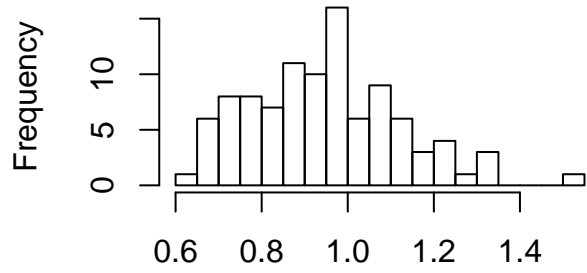


st. error of mean for theta[1]

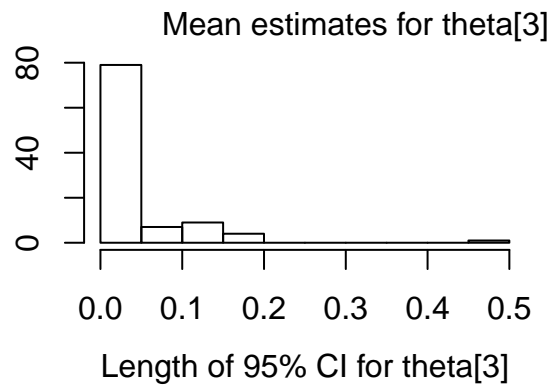
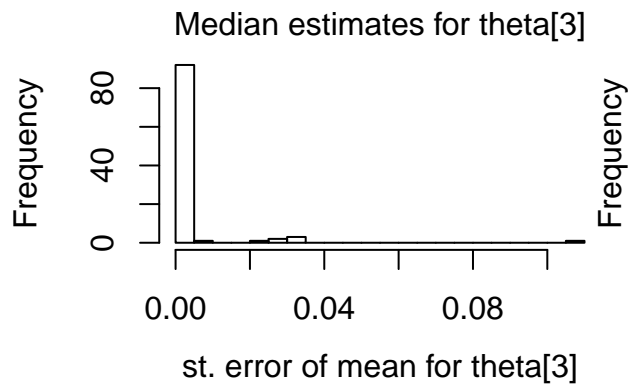
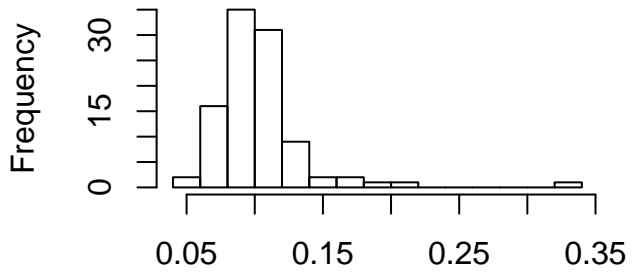
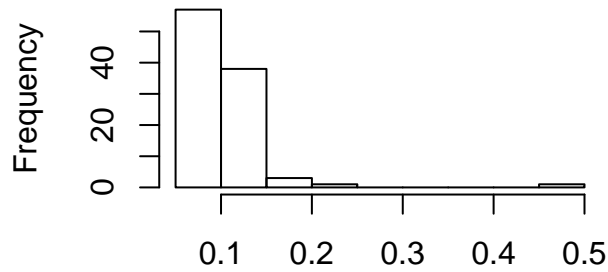


Length of 95% CI for theta[1]

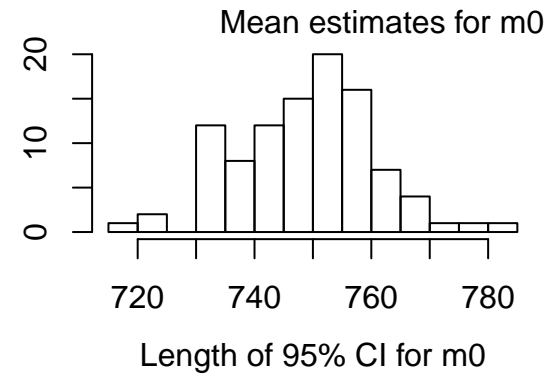
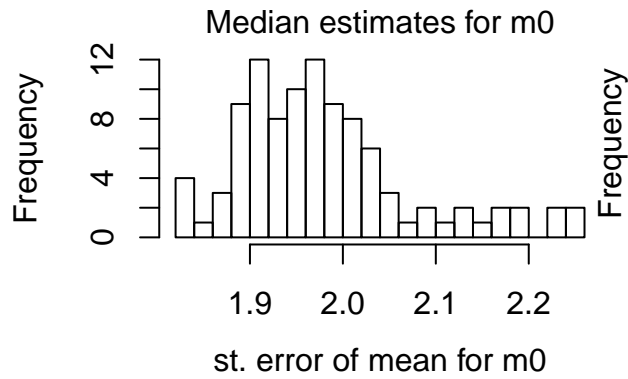
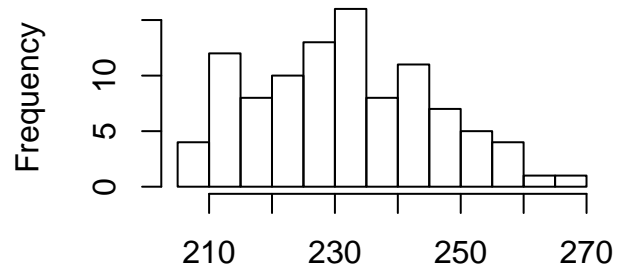
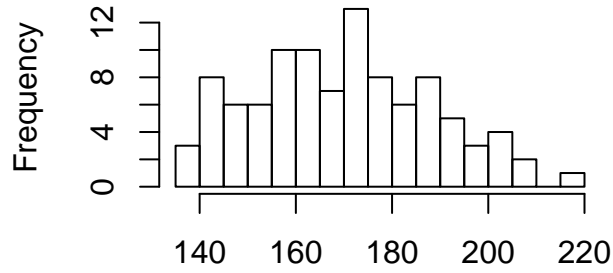
theta[2]



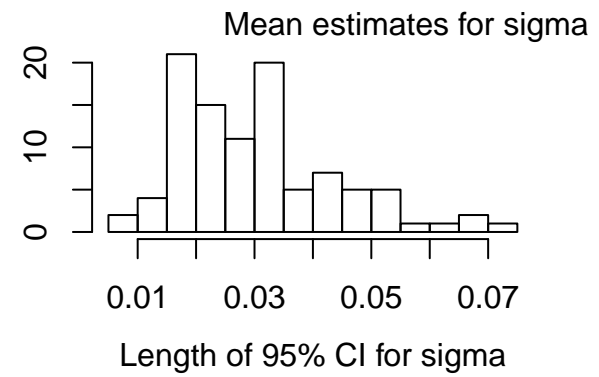
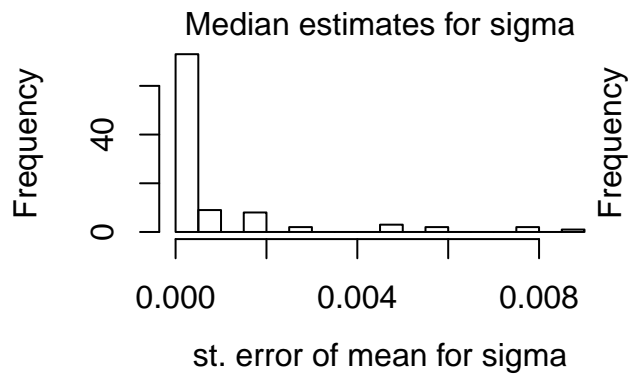
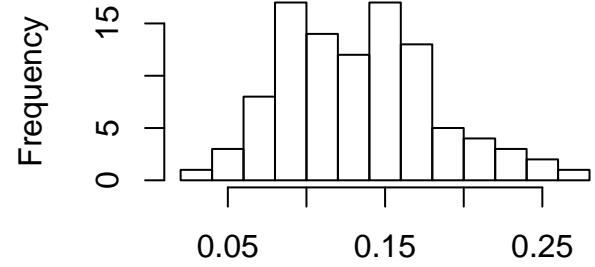
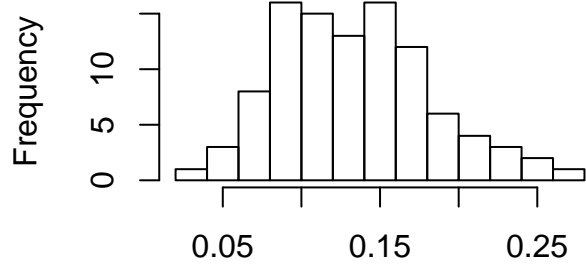
theta[3]



m0

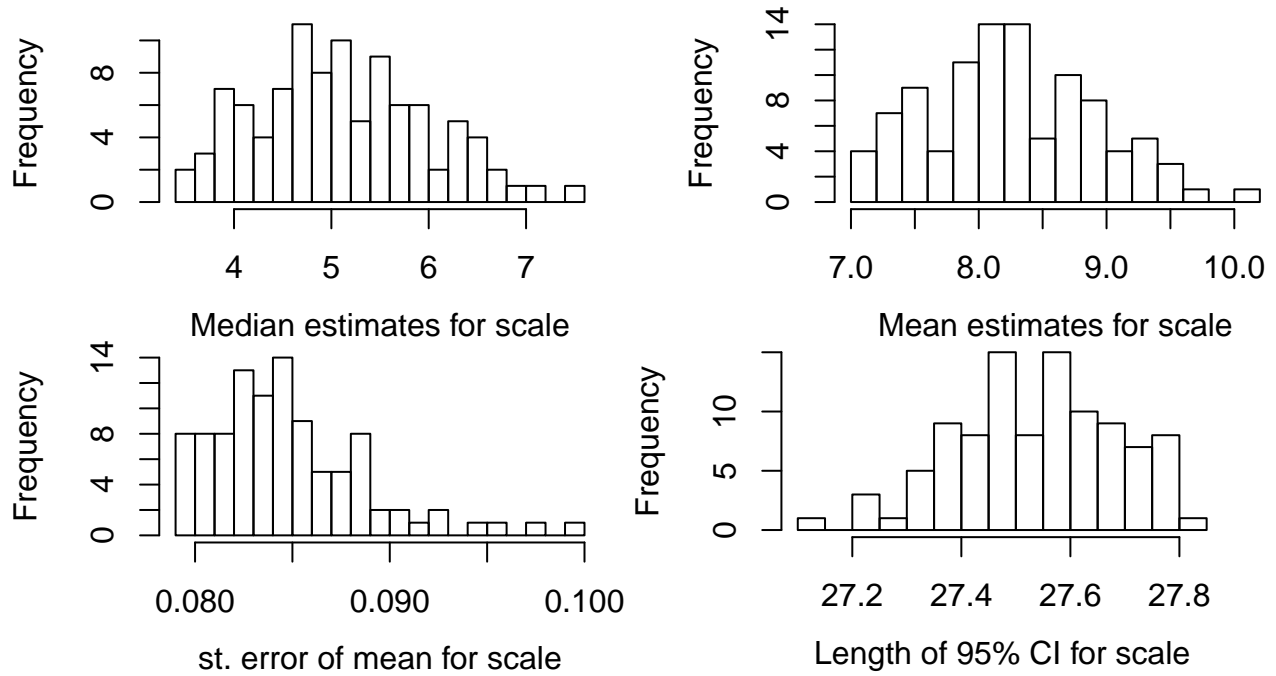


sigma

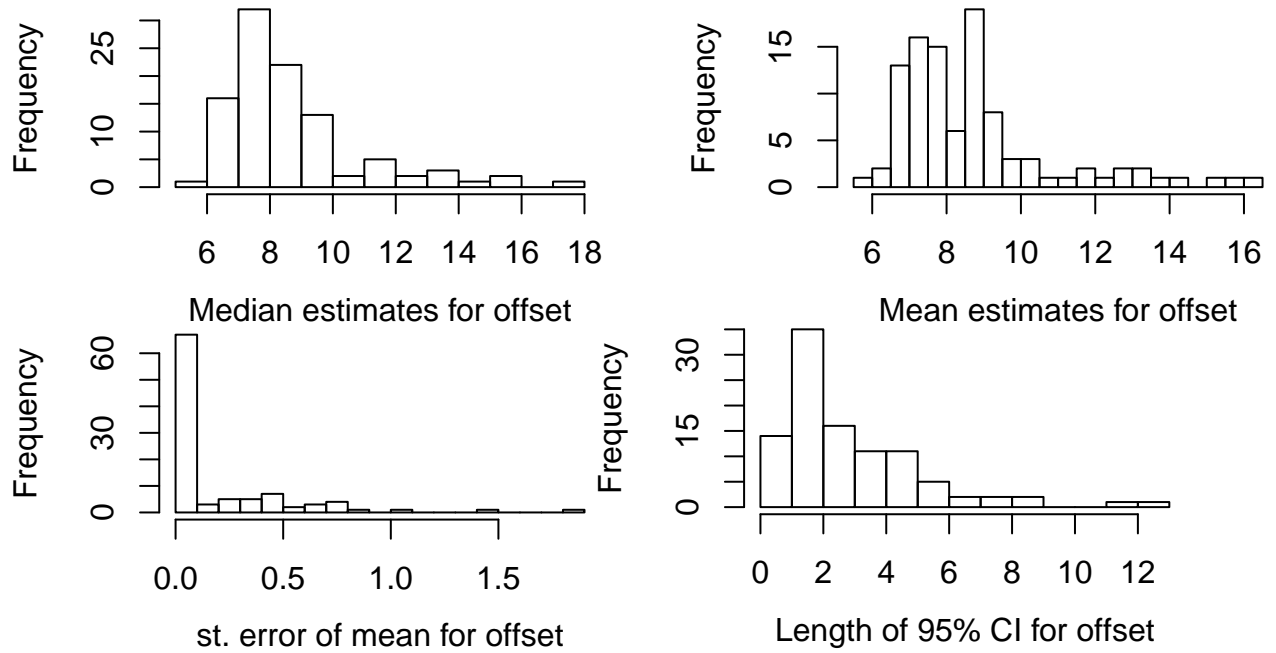




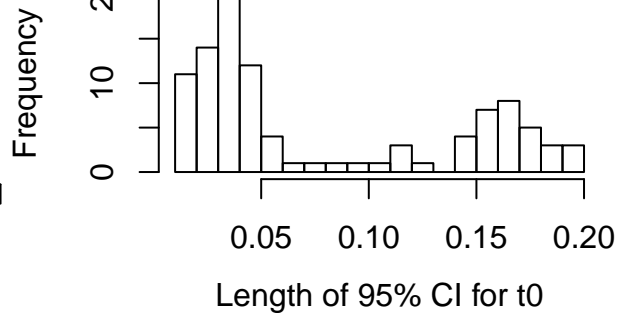
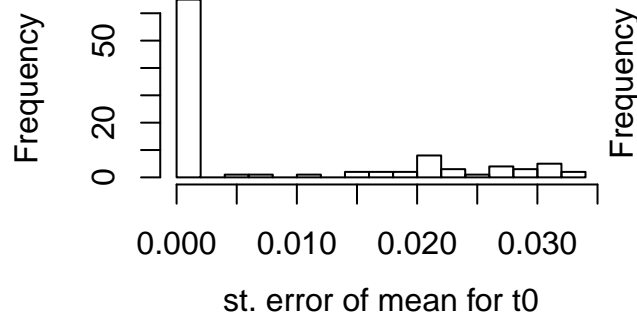
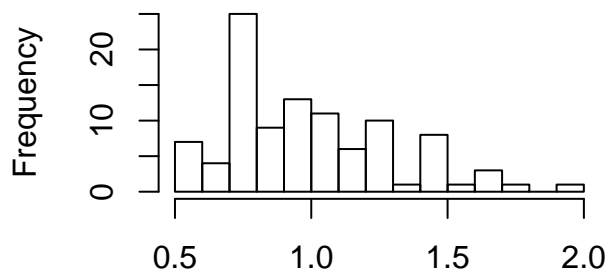
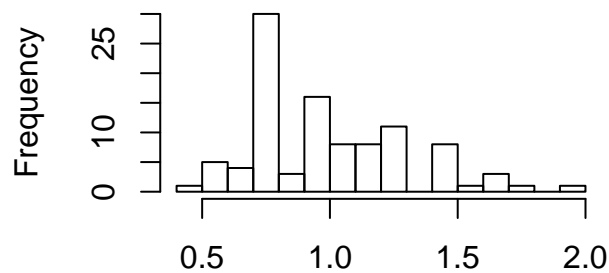
scale



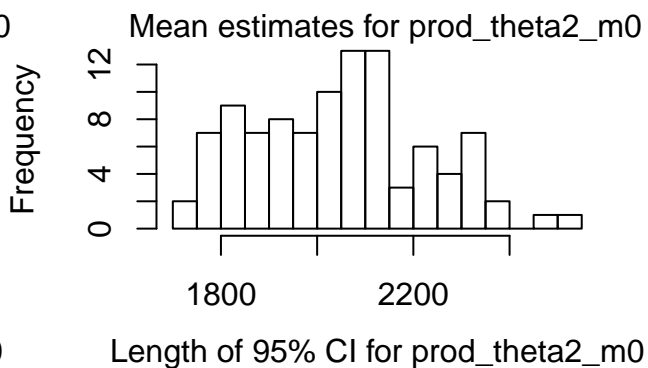
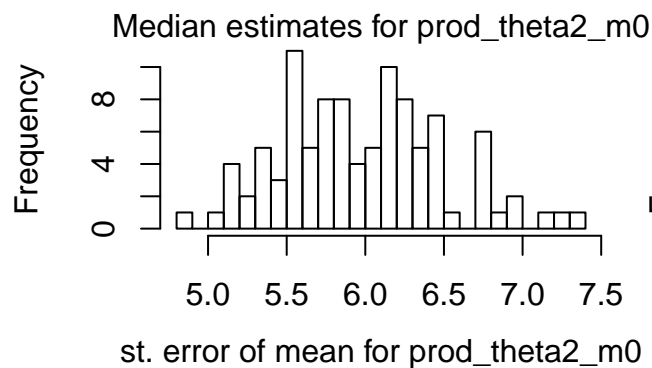
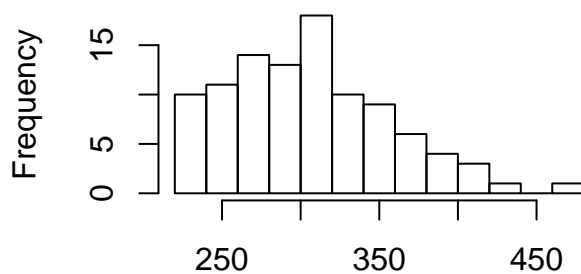
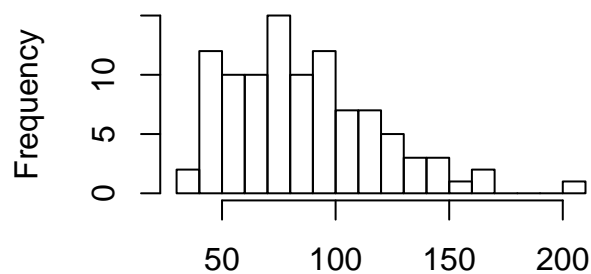
offset



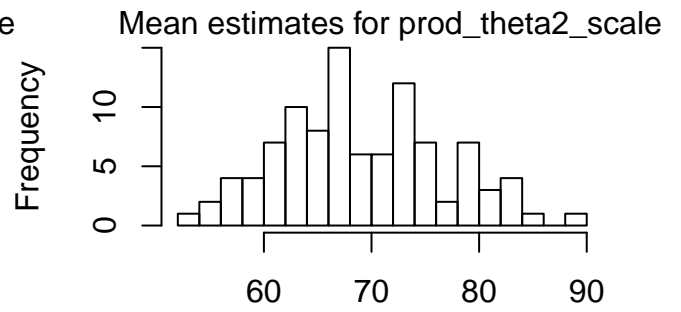
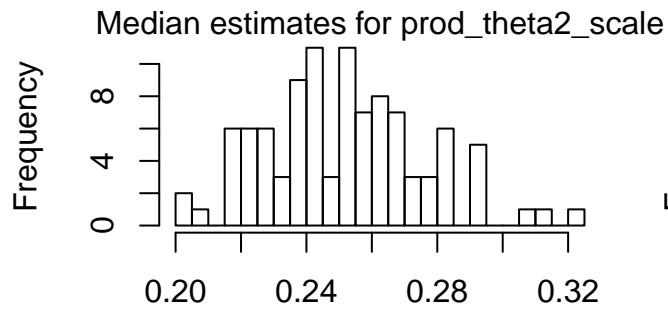
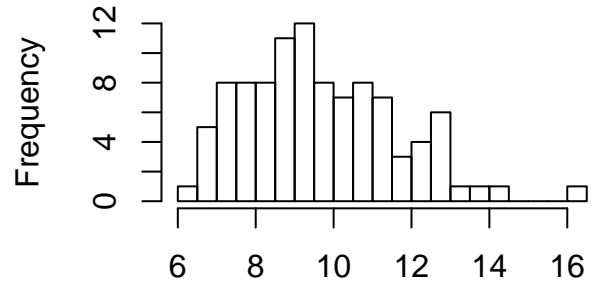
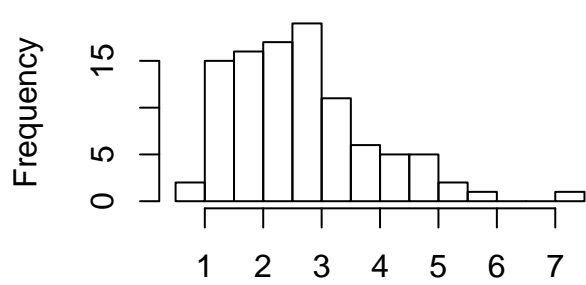
t0



prod\_theta2\_m0



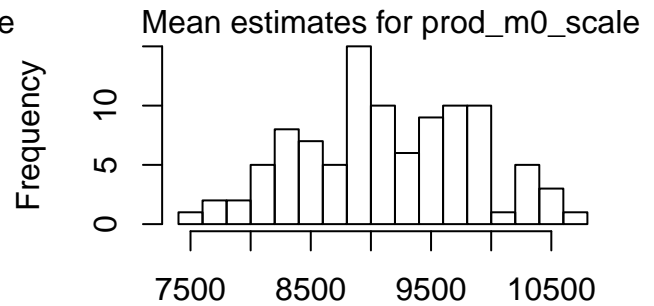
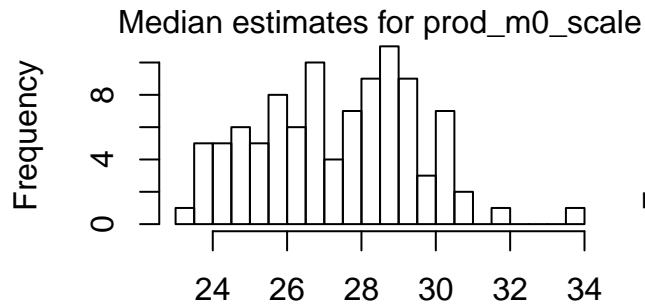
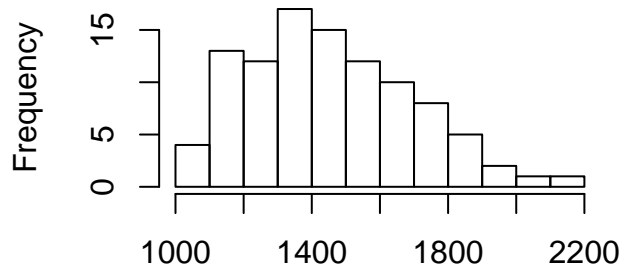
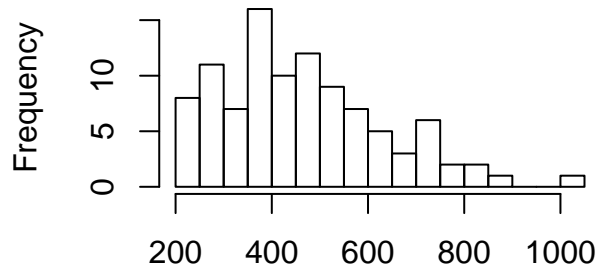
prod\_theta2\_scale



st. error of mean for prod\_theta2\_scale

Length of 95% CI for prod\_theta2\_scale

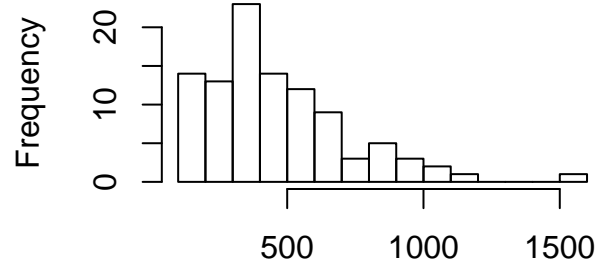
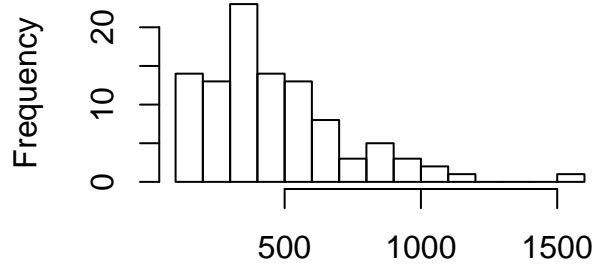
prod\_m0\_scale



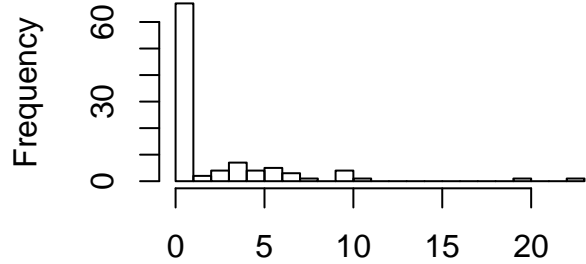
st. error of mean for prod\_m0\_scale

Length of 95% CI for prod\_m0\_scale

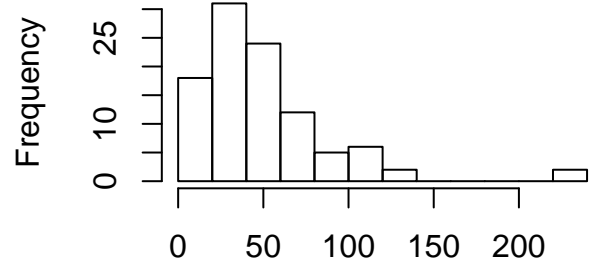
prod\_theta2\_m0\_scale



Median estimates for prod\_theta2\_m0\_scale



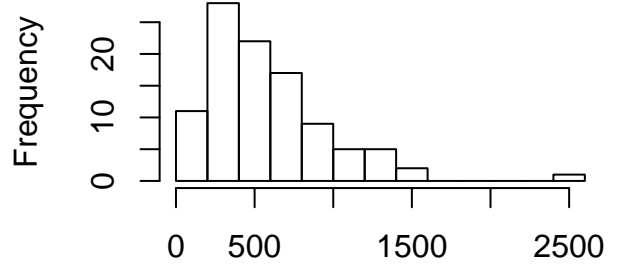
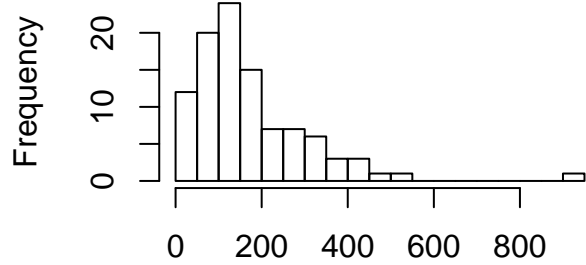
Mean estimates for prod\_theta2\_m0\_scale



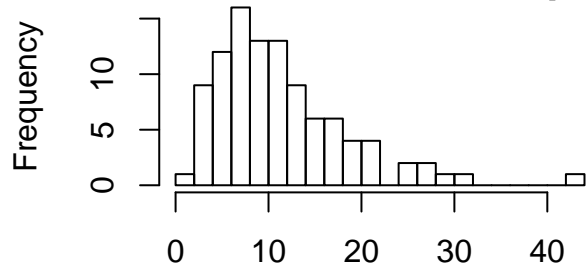
st. error of mean for prod\_theta2\_m0\_scale

Length of 95% CI for prod\_theta2\_m0\_scale

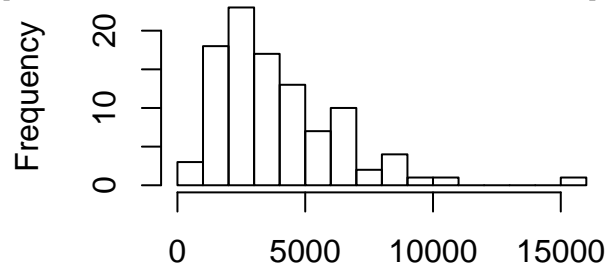
x2\_sim[180]



Median estimates for x2\_sim[180]



Mean estimates for x2\_sim[180]



st. error of mean for x2\_sim[180]

Length of 95% CI for x2\_sim[180]

## Summary of length of 95% credible intervals (CIs)

Here we give the median, standard deviation (sd), and coefficient of variation (cv) of the length of the 95% CIs.

For simulated data (where the true parameter values are known), we also give the number of times that the CI covers the true value and median, sd, and cv of the length of those 95% CIs that cover the true value.

	median_l_CI	sd_l_CI	cv_l_CI
theta[1]	0.033	0.057	1.081
theta[2]	7.880	0.213	0.027
theta[3]	0.033	0.057	1.092
m0	749.922	11.629	0.016
sigma	0.030	0.013	0.434
scale	27.551	0.147	0.005
offset	2.015	2.236	0.783
t0	0.044	0.063	0.790
prod_theta2_m0	2048.331	178.177	0.087
prod_theta2_scale	67.950	7.631	0.110
prod_m0_scale	9085.562	717.422	0.079
prod_theta2_m0_scale	40.801	38.974	0.784
x2_sim[180]	3444.914	2468.404	0.636

The following table shows the values of the median of *the length of the CIs divided by the median of each sample*

$$m_1 = \text{median} \left( \frac{q_i(0.975) - q_i(0.025)}{q_i(0.5)} \right),$$

the median of *the length of the CIs divided by the mean of each sample*

$$m_1 = \text{median} \left( \frac{q_i(0.975) - q_i(0.025)}{\text{sample\_mean}} \right),$$

as well as the median of the length of the CIs divided by *the median of the medians of the sample*

$$m_3 = \frac{\text{median}(q_i(0.975) - q_i(0.025))}{\text{median}(q_i(0.5))}.$$

and (if applicable) the median of *the length of the CIs divided by the true value*

$$m_4 = \frac{\text{median}(q_i(0.975) - q_i(0.025))}{\text{true value}}.$$

	m_1	m_2	m_3
theta[1]	0.37	0.37	0.34
theta[2]	8.38	4.35	8.32
theta[3]	0.37	0.37	0.34
m0	4.42	3.25	4.41
sigma	0.21	0.21	0.22
scale	5.46	3.35	5.46
offset	0.24	0.24	0.25
t0	0.05	0.05	0.05
prod_theta2_m0	24.39	6.76	24.58
prod_theta2_scale	27.86	7.25	27.68
prod_m0_scale	20.71	6.40	20.82
prod_theta2_m0_scale	0.10	0.10	0.10
x2_sim[180]	24.56	6.78	26.05