

MOSAIC_{bioacc} REPORT

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This report is provided by the MOSAIC_{bioacc} application available here:
<https://mosaic.univ-lyon1.fr/bioacc>

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MOSAIC_{bioacc} uses the JAGS (version 4.3.0) and R (version 4.0.2) software, and in particular packages RJags (version 4.10), jagsUI (version 1.5.1) and Shiny (version 1.6.0).

The MOSAIC_{bioacc} application is a turn-key web tool providing bioaccumulation factors (BCF/BSAF/BMF) from a toxicokinetic (TK) model fitted to accumulation-depuration data. It is designed to fulfil the requirements of regulators when examining applications for market authorization of active substances.

Data summary

File used: Apostichopus_clarithromycin_28d_Zhu2020_temperatures-variation.csv

Exposure: $10 \mu g.g^{-1}$

Accumulation phase duration: 28 days

Number of replicates: 6

Times: 0, 0.25, 0.5, 1, 2, 3, 4, 7, 10, 14.5, 15, 16, 18, 21, 24, 28, 14

Exposure routes: sediment

Elimination routes: excretion

Bayesian inference

Three MCMC chains were used to estimate model parameters.

Number of iterations: 37460

Thin: 10

TK Model

The TK model used for these calculations was:

$$\frac{dC_p(t)}{dt} = k_{us} \times c_s - (k_{ee}) \times C_p(t) \quad \text{for } 0 \leq t \leq t_c$$

$$\frac{dC_p(t)}{dt} = - (k_{ee}) \times C_p(t) \quad \text{for } t > t_c$$

with:

t : time (expressed in days)

t_c : duration of the accumulation phase (expressed in days)

$C_p(t)$: internal concentration of the parent compound at time (expressed in $\mu g.g^{-1}$)

k_{ee} : elimination rates of excretion (expressed per days $^{-1}$)

c_s : exposure concentration of sediment route (expressed in $\mu g.g^{-1}$)

k_{us} : uptake rate of sediment exposure (expressed per days $^{-1}$)

Bioaccumulation factor calculation

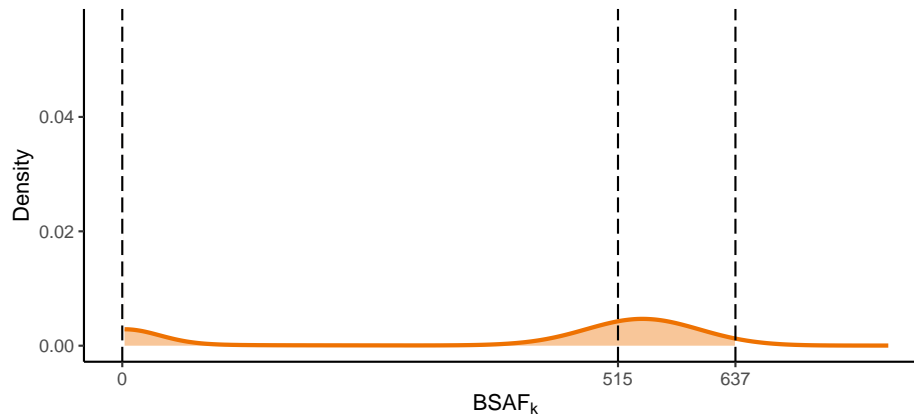
Calculations

$$BSAF_k = \frac{k_{us}}{k_{ee}}$$

$$BSAF_{ss} = \frac{C_p(t_c)}{c_s}$$

Biote-sediment accumulation factor (BSAF)

BSAF_k plot

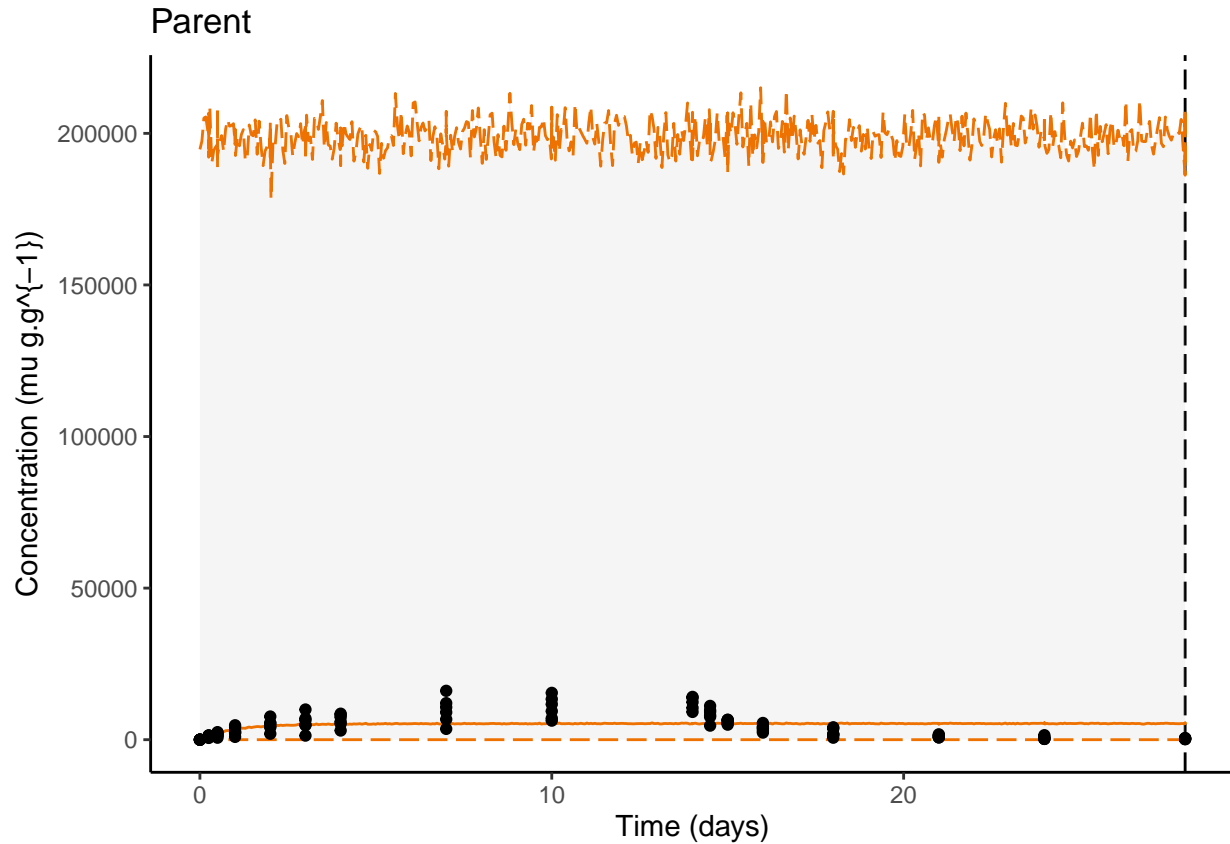


BSAF summary

	2.5%	50%	97.5%	CV
BSAFk	0	515	637	0.31

Fitting results

Fit plot



Quantiles of estimated parameters

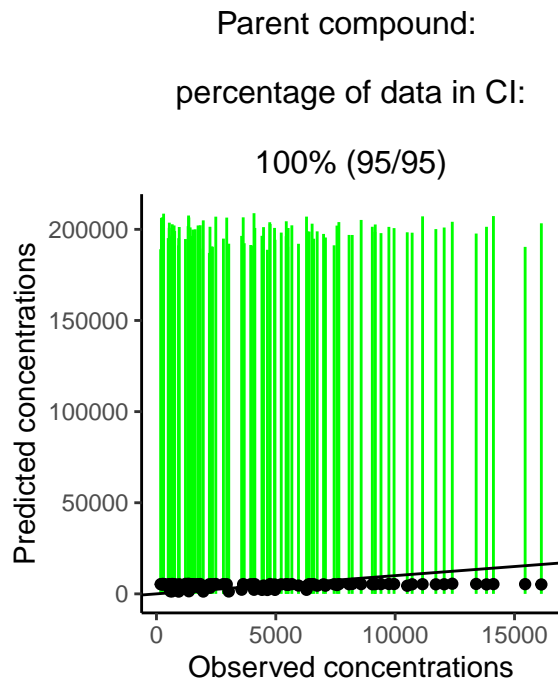
	2.5%	50%	97.5%	
k_{us}	5.086e-05	448.5	12940	d^{-1}
k_{ee}	7.787e-05	1.05	24590	d^{-1}
σ_p	3397	4043	186100	$\mu g.g^{-1}$

Goodness-of-fit criteria

Posterior Predictive Check

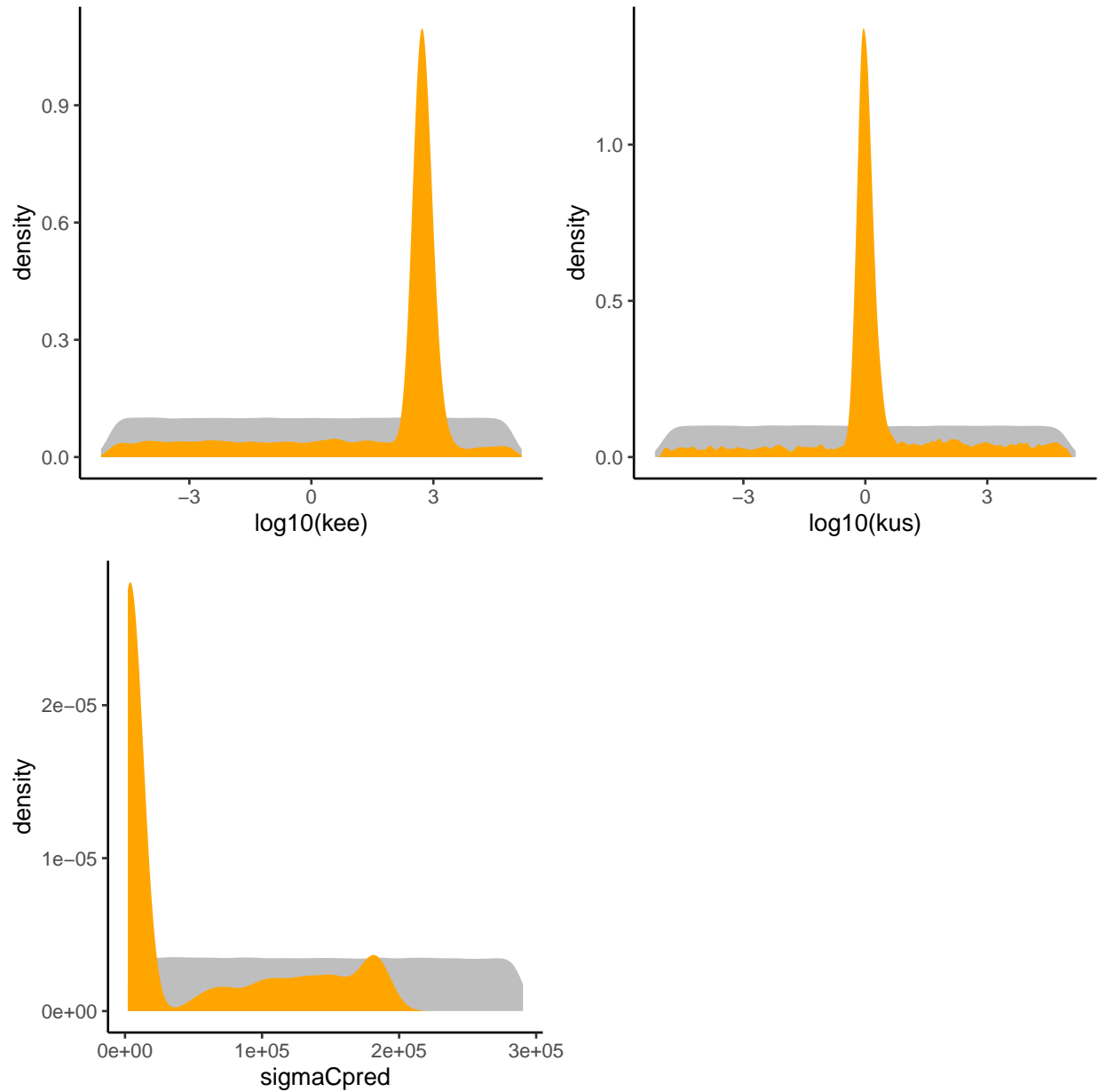
The PPC shows the observed values against their corresponding estimated predictions (black dots), along with their 95% credible interval (vertical segments). If the fit is correct, we expect to see 95% of the data within the intervals. Ideally observations and predictions should coincide, so we would expect to see black dots along the first bisector $y = x$ (plain black line). The 95% credible intervals are colored in green if they

overlap this line, in red otherwise.



Priors and posteriors

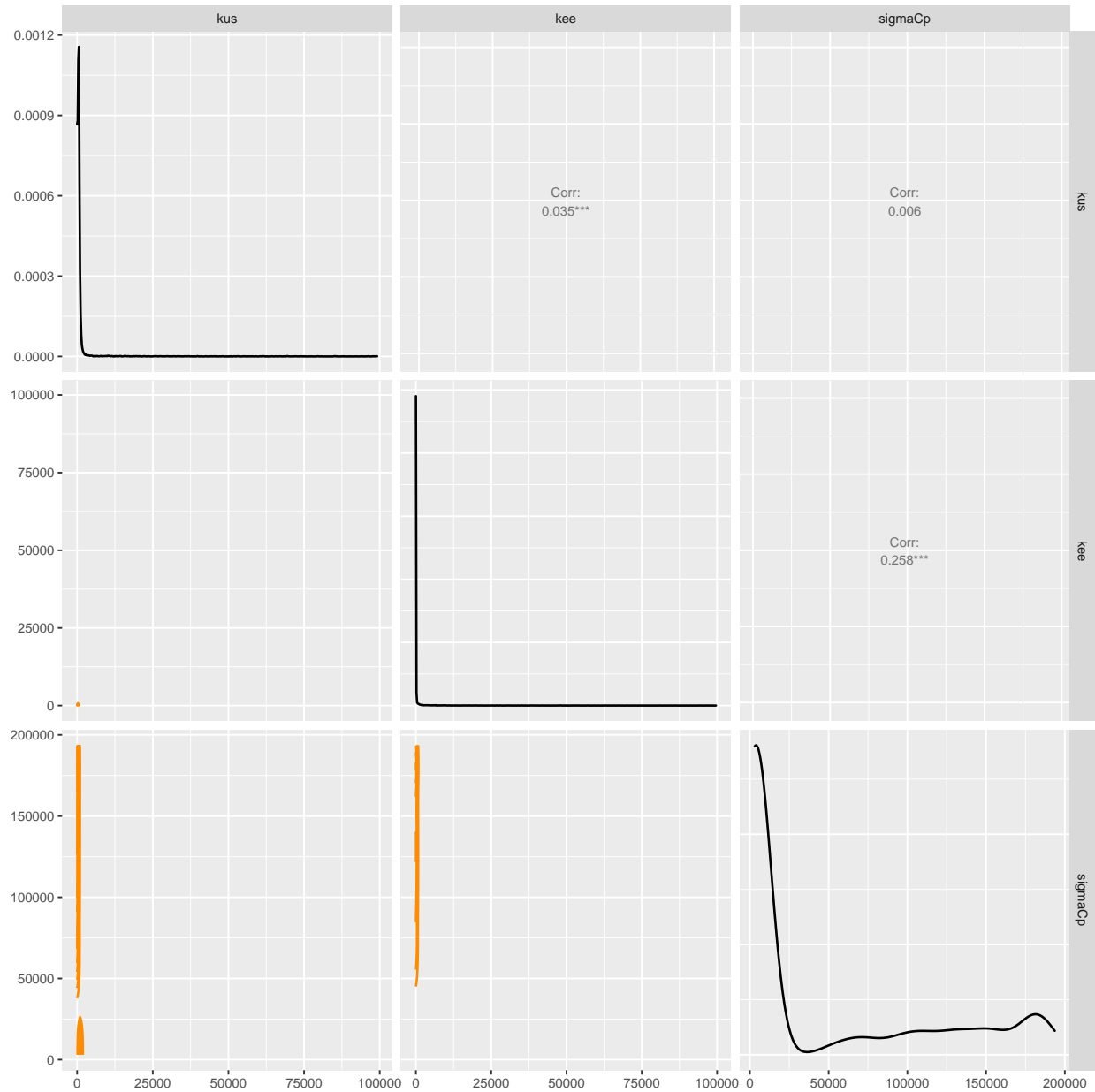
The prior distribution is represented by the gray area and the posterior distribution by the orange area. The accuracy of the model parameter estimation can be visualized by comparing prior and posterior distributions: the overall expectation is to get a narrower posterior distribution compared to the prior one, what reflects that data contributed enough to precisely estimate parameters.



Correlation between parameters

If you want to see the coloured matrix giving a summary of parameter correlations, you need to import the corresponding figure directly from the application, page bottom, section “Downloads”, then choose Download an output and select “GOF” then “parameter correlation”. You can select the output format you prefer.

Correlations between parameters are visualized by projecting the joint posterior distribution in a plot matrix with planes of parameter pairs (lower triangular elements), marginal posterior distribution of each model parameter (diagonal), and Pearson correlation coefficients (upper triangular elements). Correlations are expected to be low (reflected by “potatoid” shapes of density lines in orange); a leaning elliptical shape translates high correlations (positive if leaning to the right, negative if leaning to the left).



Potential Scale Reduction Factors

Convergence of the MCMC chains can be checked with the Gelman-Rubin diagnostic expressed with the potential scale reduction factor (PSRF). Approximate convergence is diagnosed when the PSRF is below 1.01.

	PSRF
kus	1.115688
kee	1.356744
sigmaCpred	4.703787

Watanabe–Akaike information criterion

Information criteria offer a computationally appealing way of estimating the generalization performance of the model. A fully Bayesian criterion is the widely applicable information criterion (WAIC) by Watanabe a penalized deviance statistics accounting for the uncertainty in the parameters and can be used also for singular models. WAIC is widely used in model comparison for a same dataset (e.g., with or without k_{ee}). Sub-models with lower WAIC values will be preferred.

$$\text{WAIC} = 1839$$

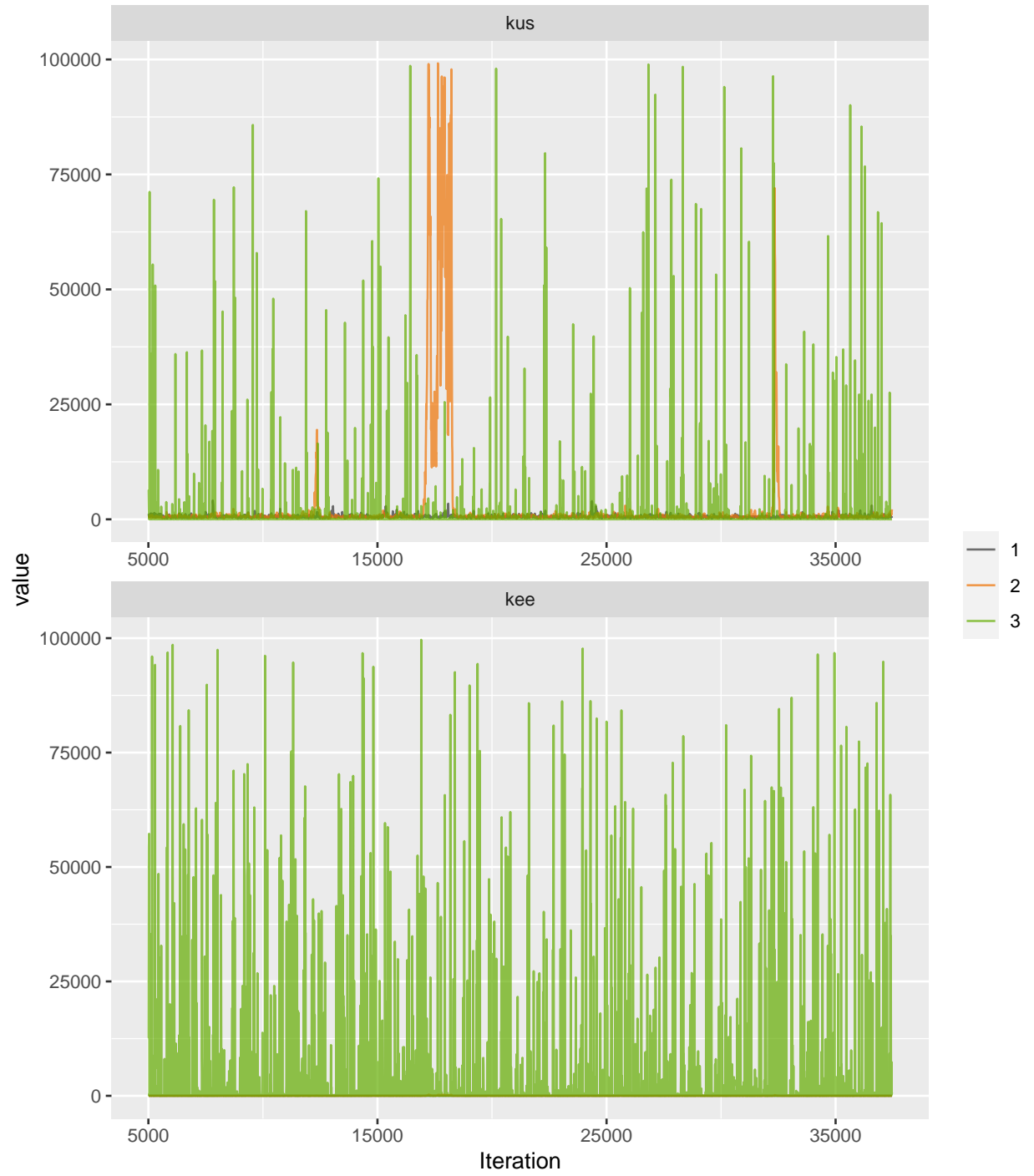
Deviance Information Criterion

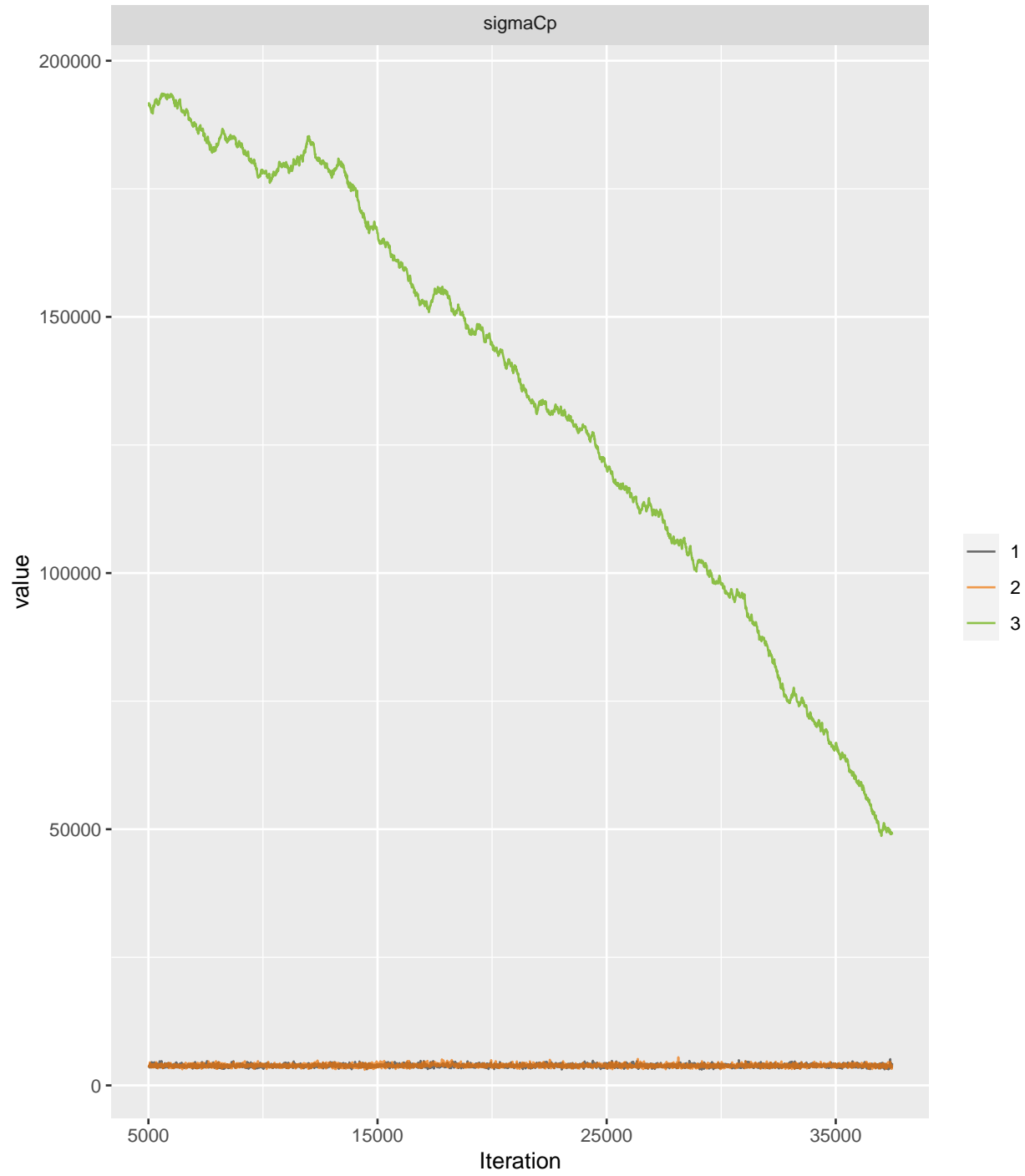
This criteria, denoted DIC, is a penalized deviance statistics accounting for the number of parameters for use in model comparison for a same dataset (e.g., with or without k_{ee}). Sub-models with lower DIC values will be preferred.

$$\text{DIC} = 2832.563$$

Traces of MCMC iterations

A traceplot is an essential plot for assessing convergence and diagnosing of MCMC chains. It shows the time series of the sampling process leading to the posterior distribution. Different colors are used for each of the chains (here 3) to assess within-chain convergence.





Data Table

time	conc	exps	replicate
0.00	0	10	1
0.25	586	10	1
0.50	656	10	1
1.00	932	10	1
2.00	1961	10	1
3.00	1358	10	1
4.00	3029	10	1
7.00	3569	10	1
10.00	6286	10	1
14.50	4646	10	1
15.00	4965	10	1
16.00	4420	10	1
18.00	4087	10	1
21.00	1772	10	1
24.00	1489	10	1
28.00	534	10	1
0.00	0	10	2
0.25	750	10	2
0.50	1362	10	2
1.00	2243	10	2
2.00	4486	10	2
3.00	4746	10	2
4.00	5950	10	2
7.00	6733	10	2
10.00	7080	10	2
14.00	10506	10	2
14.50	7562	10	2
15.00	6344	10	2
16.00	5517	10	2
18.00	3677	10	2
21.00	1400	10	2
24.00	926	10	2
28.00	493	10	2
0.00	0	10	3
0.25	1326	10	3
0.50	1818	10	3
1.00	2315	10	3
2.00	4065	10	3
3.00	4947	10	3
4.00	5227	10	3
7.00	9042	10	3
10.00	11704	10	3
14.00	9165	10	3
14.50	11148	10	3
15.00	5672	10	3
16.00	2944	10	3
18.00	1744	10	3
21.00	739	10	3
24.00	300	10	3

time	conc	exps	replicate
28.00	249	10	3
0.00	0	10	4
0.25	1216	10	4
0.50	2486	10	4
1.00	4763	10	4
2.00	5436	10	4
3.00	7000	10	4
4.00	7443	10	4
7.00	12053	10	4
10.00	13393	10	4
14.00	13826	10	4
14.50	8069	10	4
15.00	6521	10	4
16.00	2348	10	4
18.00	1624	10	4
21.00	954	10	4
24.00	268	10	4
28.00	295	10	4
0.00	0	10	5
0.25	1411	10	5
0.50	2217	10	5
1.00	4122	10	5
2.00	7642	10	5
3.00	9954	10	5
4.00	8201	10	5
7.00	16124	10	5
10.00	15445	10	5
14.00	14116	10	5
14.50	9737	10	5
15.00	5438	10	5
16.00	3949	10	5
18.00	662	10	5
21.00	764	10	5
24.00	258	10	5
28.00	208	10	5
0.00	0	10	6
0.25	1393	10	6
0.50	1522	10	6
1.00	2806	10	6
2.00	5500	10	6
3.00	6398	10	6
4.00	8575	10	6
7.00	10711	10	6
10.00	9406	10	6
14.00	12393	10	6
14.50	9152	10	6
15.00	6587	10	6
16.00	3634	10	6
18.00	1835	10	6
21.00	1346	10	6
24.00	540	10	6

time	conc	exps	replicate
28.00	177	10	6