Ecological Archives Appendices

Appendix B. Model fit and diagnostics.

For Bayesian SSMs, especially relatively complex ones such as those employed here, convergence is difficult to prove but model diagnostics are essential to reveal any major estimation flaws. For every model run we employed a number of approaches to check model convergence and fit which are detailed below.

Firstly, we examined whether the movement process model provided apparently sensible results across species. For the primary estimated parameters (γ, θ, β, m) governing the movement process model we also (i) visually inspected and applied and autocorrelation functions to the MCMC sample chains; (ii) examined the Brooks–Gelman–Rubin potential scale reduction factor ($\hat{r}$) (Brooks and Gelman 1998), using $\hat{r} \leq 1.1$ as a threshold for convergence, and (iii) assessed correlation between the posterior samples, in particular between the intercept (β_1 and β_2) and covariate coefficient (m) estimates, to check for parameter identifiability issues. For the position estimates, (iv) Geweke's simple test for convergence (Geweke 1992) was applied to all locations, and the standard Normal test sizes (Z-scores) plotted in a QQ-plot.

Visual inspection of the MCMC chains of the main model parameters revealed generally good stability and low autocorrelation within the MCMC samples for the majority of model runs. Examination of the estimated movement parameters (γ, θ, and φ) showed generally good discrimination of two movement states for the majority of model runs (Table B1). Variability across species was apparent in the relative switching probabilities (φ_1 and φ_2), with WED and SES showing the highest and lowest state transition frequencies, respectively (Table B1).

Problems were evident for WED batch 2 which estimated very similar values for γ_1 and γ_2 (Table B1). Patterns were observed in the MCMC traces and autocorrelation plots of these model runs, most commonly for γ_1, β_1 and β_2, indicating these parameters were not well resolved (Figure

B1). This batch series did not discriminate any meaningful vertical-horizontal movement relationships (refer to Table A1, Appendix A).

Problems were similarly apparent in the MCMC traces for CES batches 1 and 2, although no analogous problems were observed for batch 3. For CES batch 1 one model clearly failed to converge (run 3: examining maximum dive depth) and another (run 5: examining dive duration) again estimated very similar values for γ_1 and γ_2. States were therefore determined largely on the basis of the theta estimates, resulting in what is known as "state-flipping" (*i.e.* here state 1 = 'resident'). Interpretation of switching probabilities relative to other model runs was therefore not possible. For the remainder of runs in these batches, the most stable were those examining dive residual. Stronger wandering trends and autocorrelation was apparent in the other dive variable runs indicating poor mixing and poor resolution of parameters (in all cases for γ_1, β_2 but also in γ_1, β_1, m_1).

Excluding the problematic cases documented above, in all remaining model runs the Brooks-Gelman-Rubin diagnostic (the potential scale reduction factor: $\hat{r}$) for the intercept (β_1 and β_2) and coefficient (m) parameters governing the dive-movement relationships showed 100% of $\hat{r}$ values were ≤ 1.1 (a rule of thumb threshold for convergence). The inspection of pair-wise correlations amongst these three parameters (β_1, β_2, m) revealed high correlation ($r > 0.8$) between β_1 and m for only those model runs examining the surface residual and maximum depth dive variables, and this slope-intercept co-variability in the MCMC was not found to be associated with any other evidence of problems with model fitting.

Finally, the QQ-plots of the test sizes (z-scores) calculated from Geweke's convergence test applied to the location estimates generally showed these to be normally distributed for the majority of model runs, aside from some isolated outliers and small tails. Exceptions to this were observed in several Weddell seal runs (e.g. Figure B2), where strong departures from the normal distribution indicated some MCMC chains struggled with the estimation of a subset of positions.

Table B1. Estimates for the movement parameters (γ_i and θ_i) governing two behavioral states (where $i \in [1, 2]$ is the behavioral state index such that 1 = 'directed' (D) and 2 = 'resident' (R)) and the probabilities of switching (φ_i) between states at any time t. Note that Pr[D|D] = φ_1 hence Pr[R|D] = 1 – φ_1 whereas Pr[D|R] = φ_2 . This study uses the model formulation where φ_1 varies in relation to covariates and φ_2 is static (see Bestley et al. 2013 for process model equations). Estimate values given are the posterior mean and s.d.

			Movement parameters				Switch probabilities	
Species	Batch	Run*	γ_1	γ_2	θ_1	θ_2	$1-\varphi_1$	φ_2
SES	1	1	0.79 ± 0.02	0.36 ± 0.03	0.02 ± 0.01	3.27 ± 0.05	0.976 ± 0.022	0.024 ± 0.006
SES	1	2	0.79 ± 0.02	0.37 ± 0.03	0.02 ± 0.01	3.27 ± 0.05	0.973 ± 0.012	0.025 ± 0.006
SES	1	3	0.79 ± 0.02	0.36 ± 0.03	0.02 ± 0.01	3.27 ± 0.05	0.978 ± 0.004	0.023 ± 0.005
SES	1	4	0.79 ± 0.02	0.36 ± 0.03	0.02 ± 0.01	3.27 ± 0.05	0.978 ± 0.003	0.023 ± 0.005
SES	1	5	0.79 ± 0.02	0.36 ± 0.03	0.02 ± 0.01	3.27 ± 0.05	0.978 ± 0.004	0.023 ± 0.005
SES	2	1	0.83 ± 0.01	0.26 ± 0.05	0 ± 0.01	3.2 ± 0.08	0.971 ± 0.047	0.036 ± 0.008
SES	2	2	0.83 ± 0.01	0.28 ± 0.05	0 ± 0.01	3.2 ± 0.08	0.973 ± 0.022	0.037 ± 0.009
SES	2	3	0.83 ± 0.01	0.25 ± 0.05	0 ± 0.01	3.2 ± 0.08	0.98 ± 0.018	0.032 ± 0.008
SES	2	4	0.83 ± 0.01	0.25 ± 0.05	0 ± 0.01	3.2 ± 0.09	0.982 ± 0.003	0.03 ± 0.007
SES	2	5	0.84 ± 0.01	0.25 ± 0.05	0 ± 0.01	3.21 ± 0.08	0.976 ± 0.02	0.035 ± 0.008
SES	3	1	0.81 ± 0.02	0.44 ± 0.05	-0.01 ± 0.02	3.13 ± 0.05	0.974 ± 0.027	0.022 ± 0.006
SES	3	2	0.82 ± 0.02	0.43 ± 0.04	0 ± 0.02	3.13 ± 0.05	0.971 ± 0.021	0.022 ± 0.006
SES	3	3	0.81 ± 0.02	0.43 ± 0.05	0 ± 0.02	3.13 ± 0.05	0.976 ± 0.02	0.021 ± 0.006
SES	3	4	0.81 ± 0.02	0.43 ± 0.05	0 ± 0.02	3.13 ± 0.05	0.974 ± 0.015	0.021 ± 0.006
SES	3	5	0.82 ± 0.02	0.44 ± 0.04	0 ± 0.02	3.14 ± 0.05	0.969 ± 0.025	0.025 ± 0.007
SES	4	1	0.79 ± 0.02	0.2 ± 0.05	0 ± 0.01	3.14 ± 0.12	0.978 ± 0.023	0.024 ± 0.007
SES	4	2	0.78 ± 0.02	0.21 ± 0.05	0 ± 0.01	3.14 ± 0.12	0.98 ± 0.013	0.022 ± 0.006
SES	4	3	0.78 ± 0.02	0.19 ± 0.05	0 ± 0.01	3.14 ± 0.13	0.984 ± 0.005	0.021 ± 0.006
SES	4	4	0.78 ± 0.02	0.2 ± 0.05	0.01 ± 0.01	3.14 ± 0.12	0.984 ± 0.005	0.021 ± 0.006
SES	4	5	0.79 ± 0.02	0.2 ± 0.05	0 ± 0.01	3.15 ± 0.12	0.981 ± 0.011	0.022 ± 0.006
AFS	1	1	0.8 ± 0.03	0.04 ± 0.03	0.09 ± 0.02	2.62 ± 0.75	0.894 ± 0.007	0.159 ± 0.056
AFS	1	2	0.76 ± 0.03	0.04 ± 0.03	0.1 ± 0.03	2.8 ± 0.77	0.914 ± 0.043	0.136 ± 0.055
AFS	1	3	0.71 ± 0.04	0.04 ± 0.03	0.11 ± 0.03	2.85 ± 0.82	0.955 ± 0.02	0.088 ± 0.049
AFS	1	5	0.79 ± 0.03	0.03 ± 0.02	0.09 ± 0.03	2.77 ± 0.87	0.893 ± 0.067	0.136 ± 0.056
WED	1	1	0.72 ± 0.05	0.37 ± 0.05	-0.01 ± 0.02	3.14 ± 0.05	0.615 ± 0.094	0.181 ± 0.029
WED	1	2	0.72 ± 0.04	0.37 ± 0.05	-0.01 ± 0.02	3.13 ± 0.05	0.598 ± 0.091	0.19 ± 0.031
WED	1	3	0.72 ± 0.04	0.37 ± 0.05	-0.01 ± 0.02	3.13 ± 0.05	0.635 ± 0.006	0.176 ± 0.029
WED	1	4	0.72 ± 0.04	0.37 ± 0.05	-0.01 ± 0.02	3.13 ± 0.05	0.624 ± 0.088	0.18 ± 0.029
WED	1	5	0.72 ± 0.04	0.37 ± 0.05	-0.01 ± 0.02	3.13 ± 0.05	0.631 ± 0.026	0.179 ± 0.029
WED	2	1	0.63 ± 0.05	0.55 ± 0.03	0.05 ± 0.03	3.17 ± 0.03	0.856 ± 0.051	0.031 ± 0.011
WED	2	2	0.62 ± 0.05	0.55 ± 0.04	0.06 ± 0.03	3.17 ± 0.03	0.86 ± 0.023	0.029 ± 0.012
WED	2	3	0.64 ± 0.05	0.56 ± 0.03	0.05 ± 0.03	3.17 ± 0.03	0.812 ± 0.034	0.035 ± 0.012
WED	2	4	0.63 ± 0.05	0.55 ± 0.03	0.05 ± 0.03	3.17 ± 0.03	0.829 ± 0.008	0.034 ± 0.013
WED	2	5	0.64 ± 0.05	0.56 ± 0.03	0.05 ± 0.03	3.17 ± 0.03	0.816 ± 0.025	0.035 ± 0.013

WED	3	1	0.74 ± 0.03	0.5 ± 0.04	-0.04 ± 0.02	3.14 ± 0.03	0.598 ± 0.104	0.156 ± 0.021
WED	3	2	0.74 ± 0.03	0.5 ± 0.04	-0.04 ± 0.02	3.14 ± 0.03	0.589 ± 0.113	0.157 ± 0.021
WED	3	3	0.75 ± 0.04	0.5 ± 0.04	-0.04 ± 0.02	3.14 ± 0.03	0.616 ± 0.07	0.149 ± 0.02
WED	3	4	0.75 ± 0.03	0.5 ± 0.04	-0.04 ± 0.02	3.14 ± 0.03	0.636 ± 0.032	0.144 ± 0.02
WED	3	5	0.75 ± 0.04	0.5 ± 0.04	-0.04 ± 0.02	3.14 ± 0.03	0.606 ± 0.071	0.153 ± 0.021
WED	4	1	0.8 ± 0.04	0.56 ± 0.03	0.01 ± 0.02	3.15 ± 0.04	0.814 ± 0.084	0.027 ± 0.006
WED	4	2	0.8 ± 0.04	0.56 ± 0.03	0.01 ± 0.02	3.15 ± 0.04	0.771 ± 0.097	0.03 ± 0.007
WED	4	3	0.78 ± 0.04	0.57 ± 0.03	0.01 ± 0.02	3.14 ± 0.04	0.809 ± 0.056	0.027 ± 0.006
WED	4	4	0.79 ± 0.04	0.56 ± 0.03	0.01 ± 0.02	3.15 ± 0.04	0.836 ± 0.011	0.026 ± 0.006
WED	4	5	0.79 ± 0.04	0.56 ± 0.03	0.01 ± 0.02	3.15 ± 0.04	0.812 ± 0.046	0.028 ± 0.006
CES	1	1	0.63 ± 0.05	0.19 ± 0.07	0.1 ± 0.06	3.23 ±0.27	0.958 ± 0.01	0.013 ± 0.007
CES	1	5	0.39 ± 0.05	0.41 ± 0.05	0.3 ± 0.08	2.45 ±0.15	0.973 ± 0.041	0.032 ± 0.015
CES	2	1	0.63 ± 0.07	0.22 ± 0.09	0.03 ± 0.06	3.24 ±0.31	0.965 ± 0.016	0.02 ± 0.012
CES	2	3	0.62 ± 0.06	0.17 ± 0.09	0.04 ± 0.06	3.3 ±0.37	0.979 ± 0.012	0.014 ± 0.011
CES	2	5	0.66 ± 0.07	0.18 ± 0.08	0.03 ± 0.06	3.27 ±0.34	0.949 ± 0.08	0.023 ± 0.013
CES	3	1	0.69 ± 0.05	0.14 ± 0.06	0.02 ± 0.04	3.28 ±0.32	0.883 ± 0.051	0.045 ± 0.018
CES	3	3	0.7 ± 0.06	0.13 ± 0.06	0.02 ± 0.05	3.31 ±0.35	0.883 ± 0.016	0.043 ± 0.018
CES	3	5	0.7 ± 0.06	0.13 ± 0.06	0.02 ± 0.05	3.28 ±0.35	0.864 ± 0.058	0.048 ± 0.021

*Run refers here to the dive variable examined where: 1 = ‘dive residual’; 2 = ‘surface residual’; 3 = maximum dive depth; 4 = bottom time; 5 = dive duration.

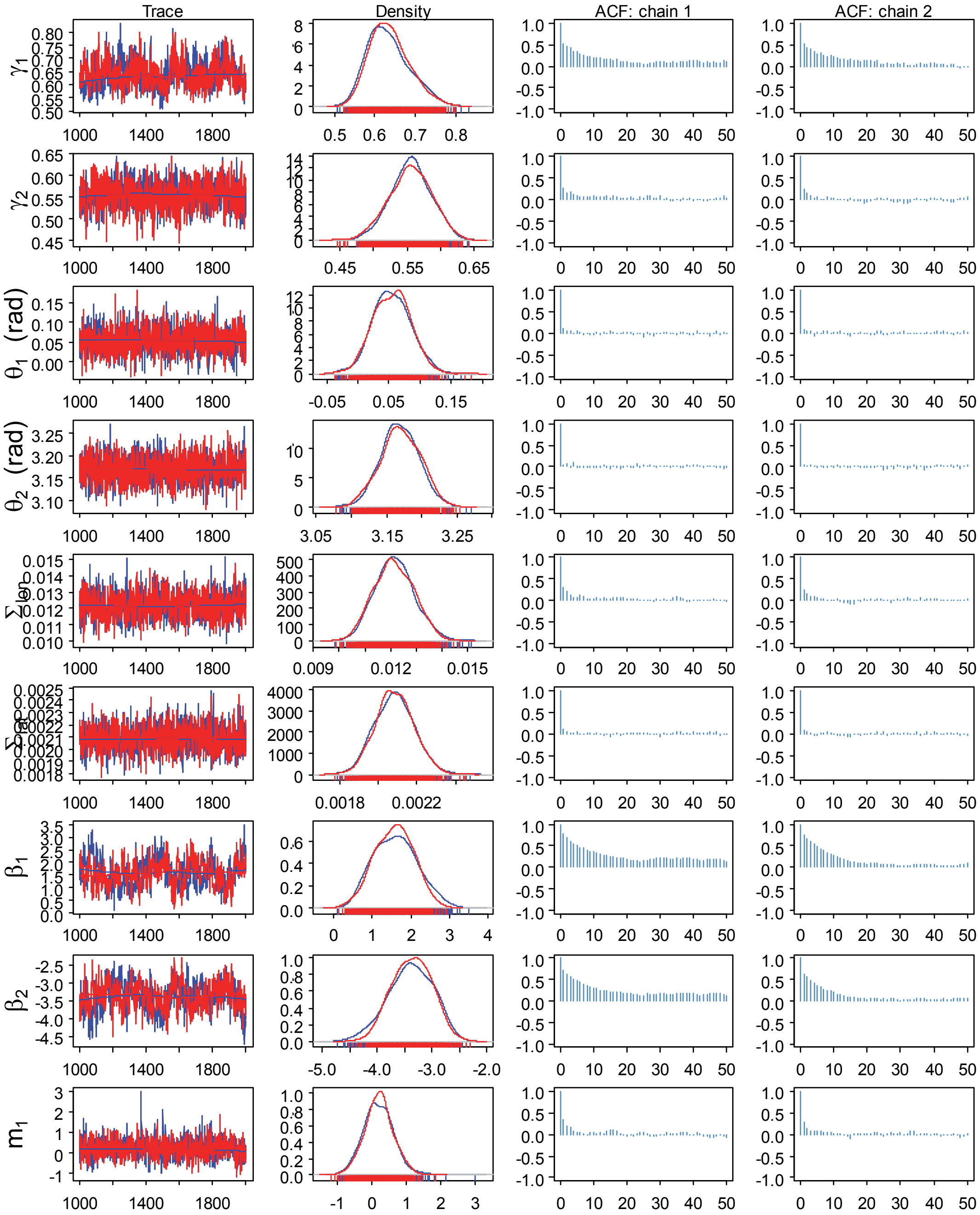

Figure B1. Example diagnostic summary showing problematic model fit for Weddell seal batch 2 (model run 5: examining dive duration). Each row contains: a trace plot of the thinned chains, density plot of the thinned chains, auto-correlation function of the thinned chains. Failure to discriminate well between γ_1 and γ_2 results in poor ability to identify the intercept parameters governing switching between movement states (β_1 and β_2), and no resolution of the covariate coefficient ($m_1 \sim 0$).

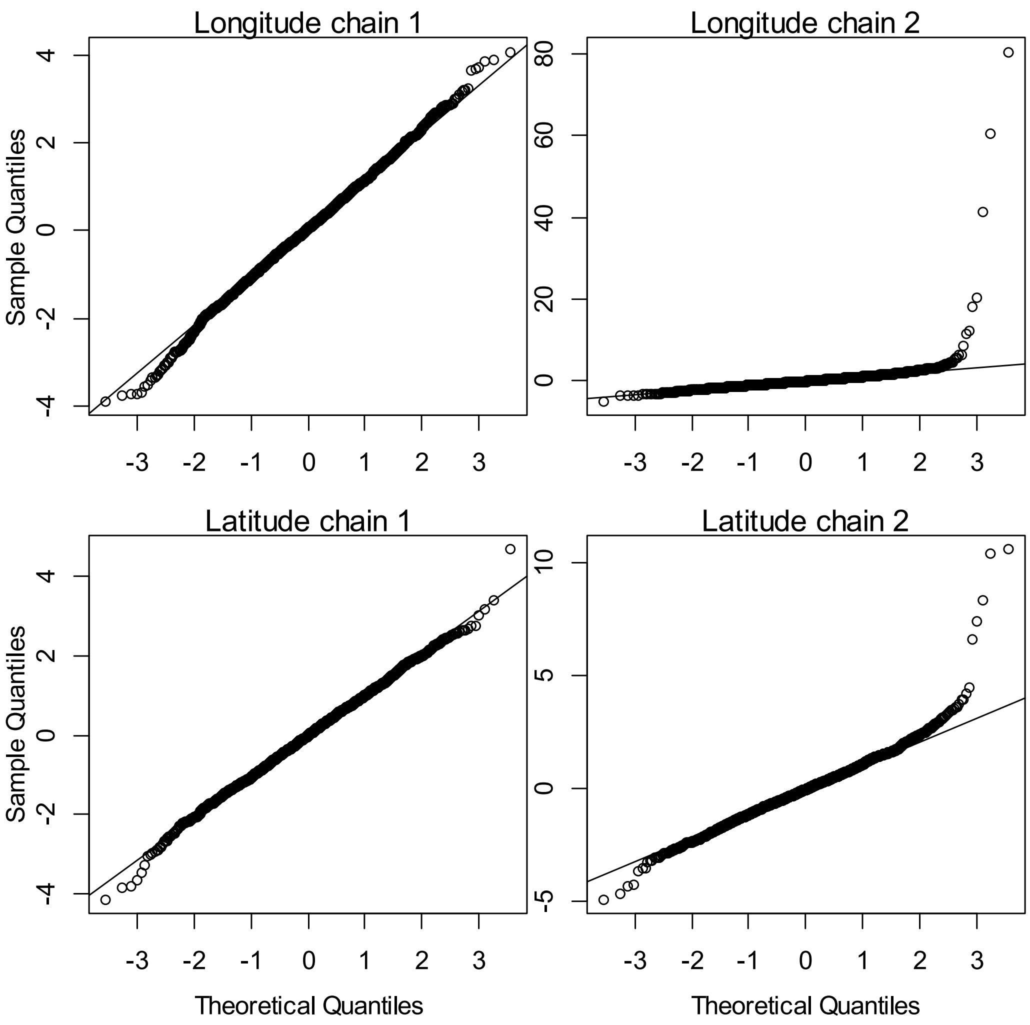

Figure B2. QQ-plots of the test sizes (z-scores) calculated from Geweke's convergence test of the MCMC chains for estimated positions (2715 longitudes and latitudes), using a Weddell seal example (batch 4 run 3: examining maximum dive depth). Points should lie on the line with intersect 0 and slope 1, which is not the case here for chain 2.

References

Bestley, S., I. D. Jonsen, M. A. Hindell, C. Guinet, and J. B. Charrassin. 2013. Integrative modelling of animal movement: incorporating in situ habitat and behavioural information for a migratory marine predator. Proceedings of the Royal Society B-Biological Sciences **280**:22262-22262.

Brooks, S. P. and A. Gelman. 1998. General methods for monitoring convergence of iterative simulations. Journal of Computational and Graphical Statistics **7**:434-455.

Geweke, J. 1992. Evaluating the accuracy of sampling-based approaches to calculating posterior moments.*in* J. M. Bernado, J. O. Berger, A. P. Dawid, and A. F. M. Smith, editors. Bayesian Statistics 4. Clarendon Press, Oxford, UK.