

Supplementary Appendix

Full inference of distance-based models

Bayesian inference also allows us to estimate both parameters, γ and σ , simultaneously. The ensemble obtained with free parameters appears to be the blurred version of the ensemble with fixed data weight (see Fig. A1 for a comparison of the average distance matrices). The parameters of the lognormal model are shown in Figure A2. Both γ and the weight $w = 1/\sigma^2$ are estimated to be smaller compared to the values obtained with fixed w . Figure A3 shows a comparison of the energies, log likelihoods, radii of gyration and other quantities for the simulation with fixed and variable σ .

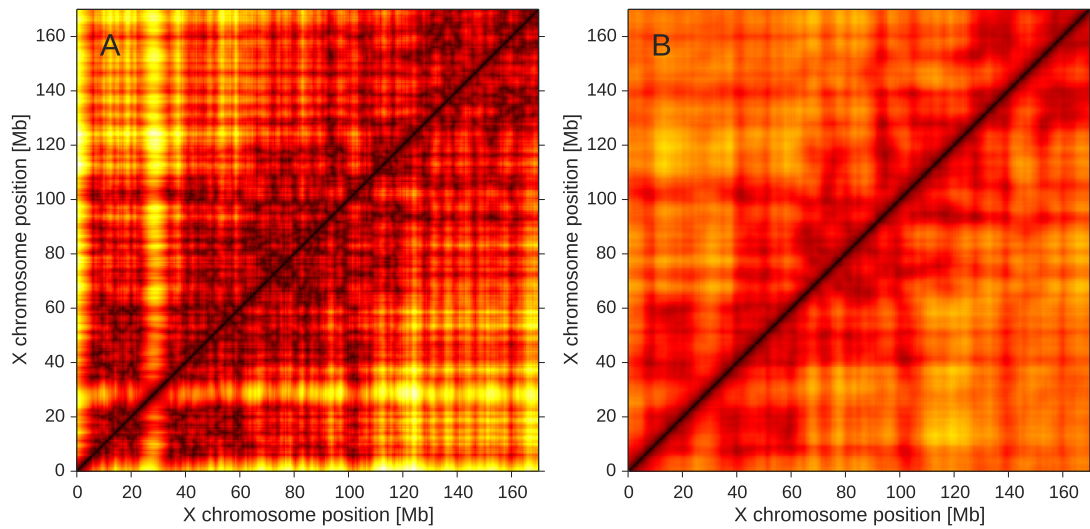


Fig A1: Comparison of distance-based structure ensembles assuming a lognormal error model. **(A)** Average distance matrix with fixed data weight $w = \sigma^{-2} = 500$. **(B)** Average distance matrix with free $w = \sigma^{-2}$ and distance scale γ .

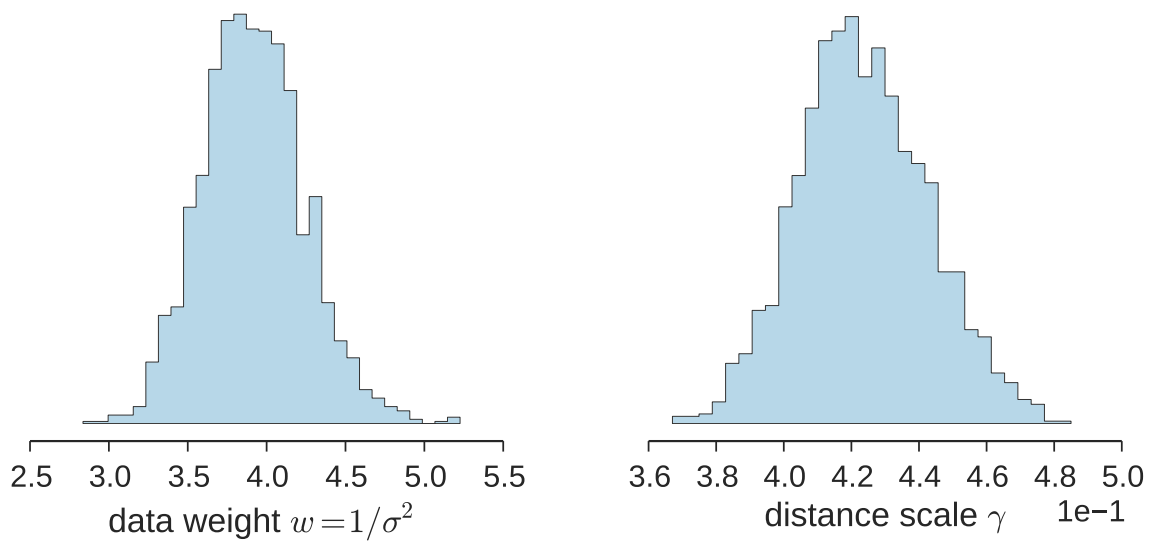


Fig A2: Estimated model parameters for the lognormal model.

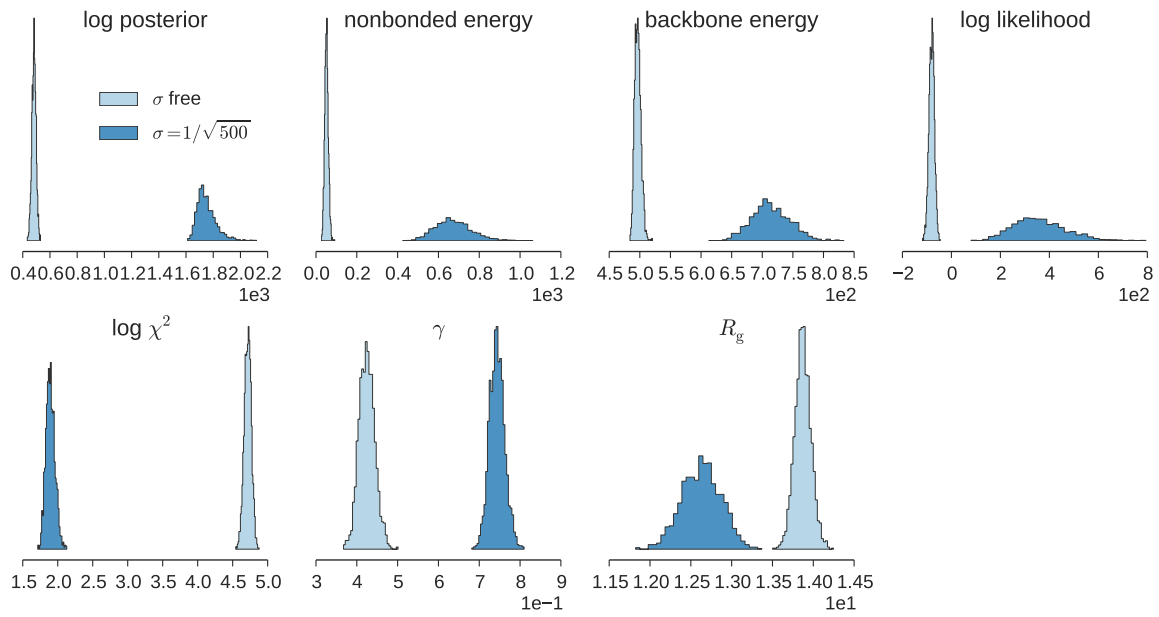


Fig A3: Comparison of ensembles calculated with fixed and variable data weight σ^{-2} .