
Supplementary information

A flexible Bayesian framework for unbiased estimation of timescales

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Supplementary Information for: A flexible Bayesian framework for unbiased estimation of timescales

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Supplementary Tables

Figures	Data parameters
Fig. 3a, Fig. 5a	$\tau = 20, \mu = 0, \sigma = 1$
Fig. 3b	$\tau = 60, f = 2 \text{ Hz}, \mu = 0, \sigma = 1$
Fig. 3c, Fig. 5d	$\tau_1 = 5, \tau_2 = 80, c_1 = 0.4, \mu' = 1, \sigma' = 0.5$
Fig. 5g	$\tau_1 = 20, \tau_2 = 80, c_1 = 0.4, \mu' = 0.3, \sigma' = 0.18$

Supplementary Table 1. Simulation parameters for data autocorrelations.

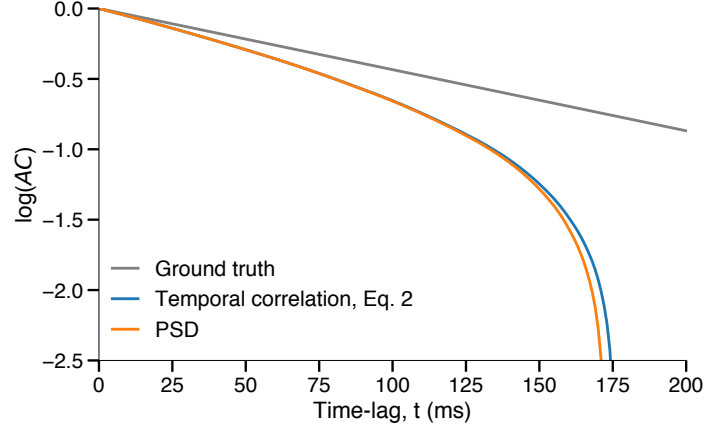
Figures	Priors	t_m
Fig. 3a, Fig. 4, Fig. 5b	$\tau, \tau_1, \tau_2 : U[0, 60]$	50
Fig. 3b	$\tau : U[0, 120]$	100
Fig. 3c, Fig. 5e (Right)	$\tau_1 : U[0, 60], \tau_2 : U[20, 140]$	110
Fig. 5e (Left)	$\tau : U[0, 140]$	110
Fig. 5h (Right)	$\tau_1 : U[0, 60], \tau_2 : U[40, 150]$	105
Fig. 5h (Left)	$\tau : U[0, 150]$	105
Fig. 6b	$\tau_1 : U[0, 60], \tau_2 : U[40, 150]$	150
Fig. 6a	$\tau : U[0, 150]$	150

Supplementary Table 2. aABC fit parameters. $U[a, b]$ denotes a uniform distribution on the interval $[a, b]$.

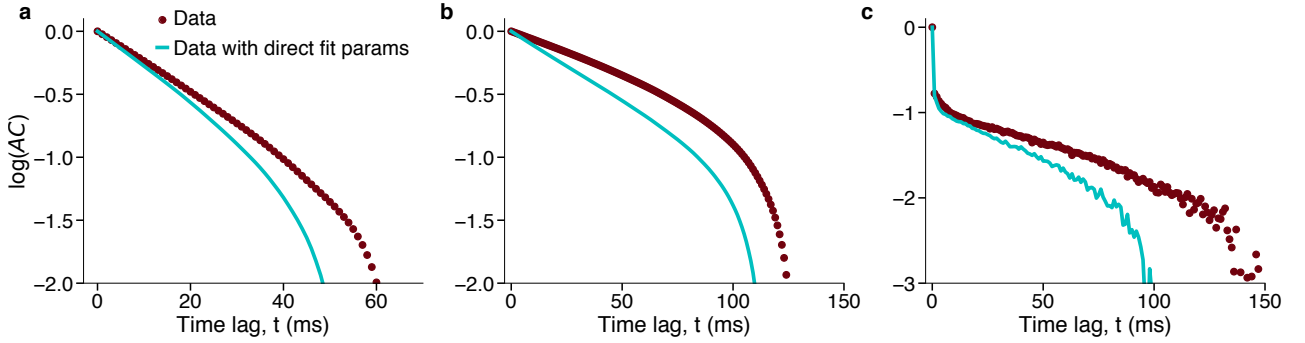
Generative model	Number of trials	Number of posterior samples	Run time (min)
One-timescale OU (1 parameter)	100	100	5
One-timescale OU (1 parameter)	500	100	20
One-timescale OU (1 parameter)	100	500	23
Two-timescale OU (3 parameters)	100	100	6
One-timescale OU and two oscillations (5 parameters)	100	100	7

Supplementary Table 3. Running time of the aABC algorithm using the PSD as the summary statistic and 20 parallel processors (Intel(R) Xeon(R) Gold 6152 CPU @ 2.10GHz). Trial duration is 1 sec.

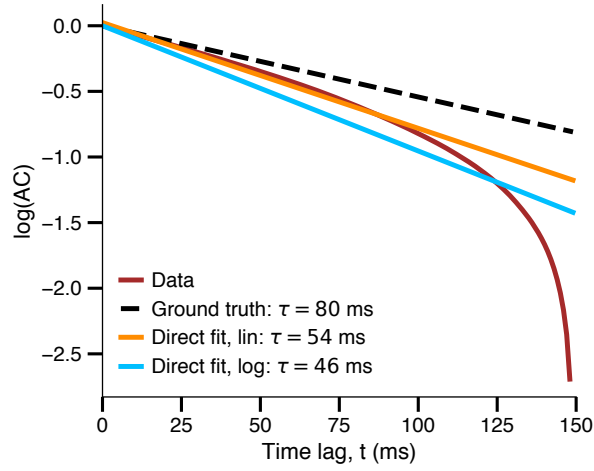
Supplementary Figures



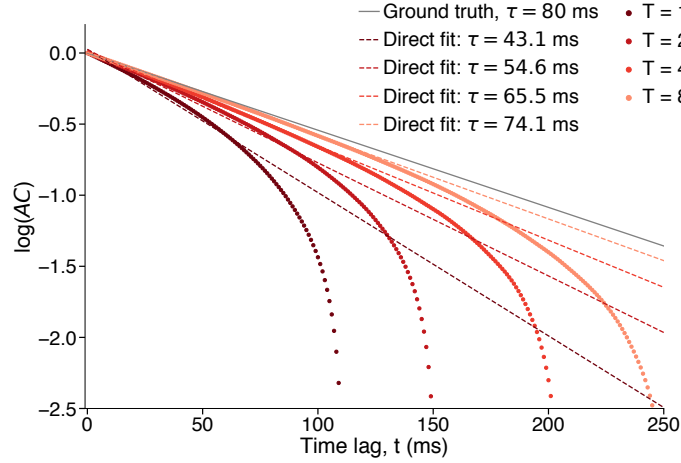
Supplementary Figure 1. Bias in the sample autocorrelation computed from different methods due to finite data. Computing autocorrelations in the time domain (equation (2), blue) or via the inverse Fourier transform of the PSD (orange) both produce biased results. Data are generated from an OU process with the timescale $\tau = 100$ ms and duration $T = 1$ s. Autocorrelations are averaged over 500 trials (realizations). PSDs are computed after applying a Hamming window to each trial.



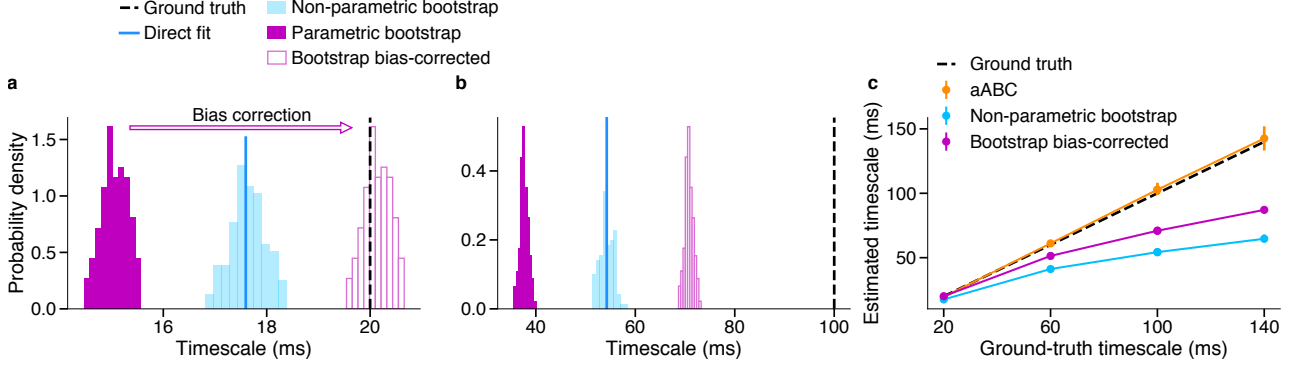
Supplementary Figure 2. Negative bias in autocorrelation of synthetic data with direct fit parameters. Autocorrelation of synthetic data (cyan) generated with parameters estimated by direct fit deviates from the autocorrelation of the original fitted data (brown). The same synthetic data as in Fig. 1, middle, from a-c respectively. The synthetic data are generated from the correct functional form of generative models with the same statistics (e.g., duration and number of trials) as in the observed data, using parameters obtained from direct exponential fits to observed data autocorrelations.



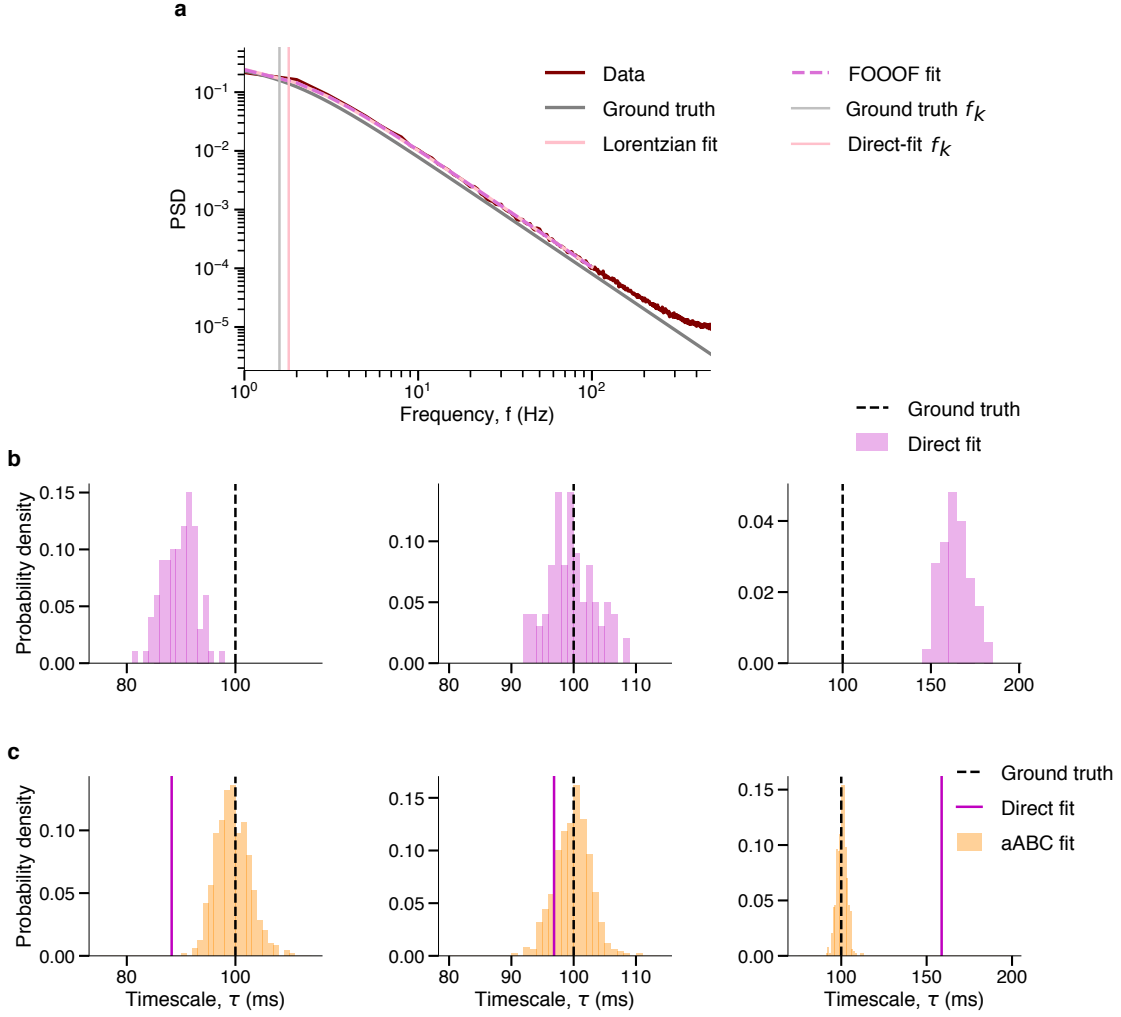
Supplementary Figure 3. Larger estimation errors in direct fitting the autocorrelation shape in logarithmic-linear space than in linear space. The estimated timescale from fitting the sample autocorrelation shape with an exponential decay function is more biased when using logarithmic distances (blue line) than using linear distances (orange line), since it puts more emphasis on the autocorrelation tail which is more affected by the bias (larger deviations between the autocorrelations of data and the ground truth). For a fair comparison between logarithmic and linear fits, only positive correlation values are included in the fitting. Data consists of 500 trials that are generated from an OU process with the timescale $\tau = 80$ ms and duration $T = 1$ s.



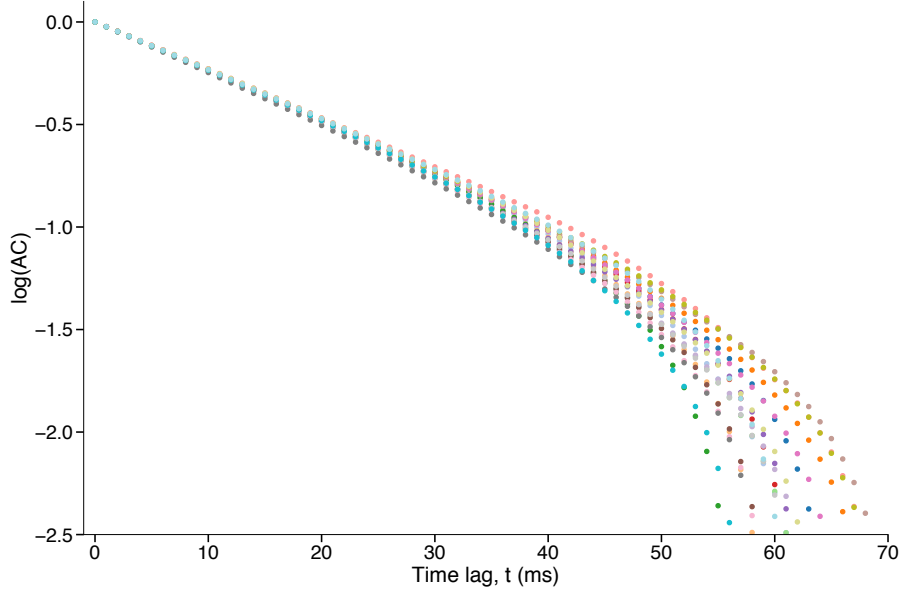
Supplementary Figure 4. Impact of trial duration on estimated timescales from direct fitting. Direct exponential fit produces different estimated timescale for datasets from the same generative process but with different trial duration. Each dataset is generated from an OU process with $\tau = 80$ ms and 500 trials each with duration T . Dots - sample autocorrelation, dashed lines - direct exponential fit, solid line - ground truth.



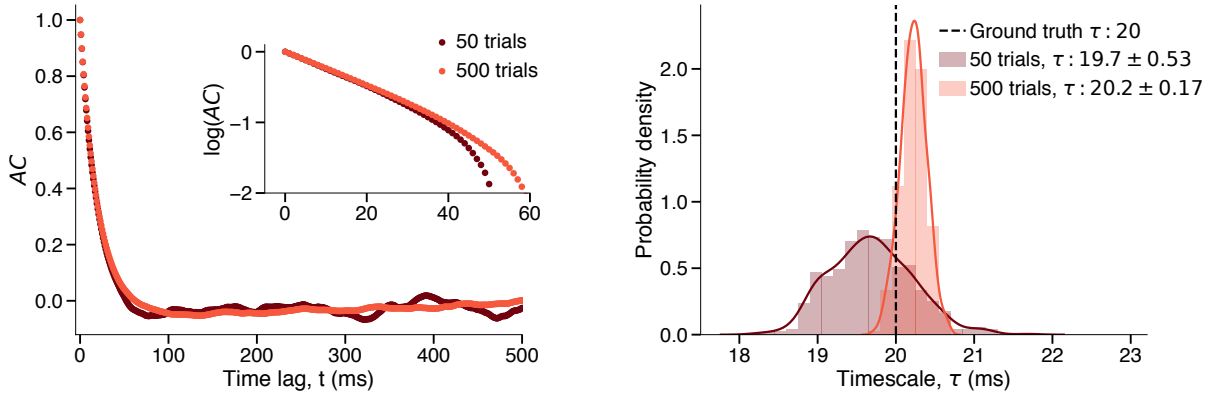
Supplementary Figure 5. Bootstrapping for the uncertainty estimation and bias correction. (a-b) Using bootstrapping for the bias correction does not guarantee unbiased estimation of timescales, since the amount of bias depends on the ground-truth timescale. Data are generated from an OU process with a given ground-truth timescale (dashed line, 500 trials with $T = 1$ s duration). Directly fitting the average autocorrelation shape with an exponential decay function underestimates the timescale (blue line). For parametric bootstrapping, we generate 100 synthetic datasets from an OU process with the timescale estimated by the direct fit and other statistics (e.g., duration and number of trials) as in the original data. We estimate the timescale from each synthetic dataset again with a direct exponential fit (magenta filled bars distribution). The difference between the mean of bootstrapping distribution and the original direct fit estimate can be used as an offset to correct the bias (magenta empty bars distribution). The variance of bootstrapping distribution provides a measure of uncertainty. However, this method only works for some cases (a) and does not guarantee an unbiased estimate for every case (b). For non-parametric bootstrapping, we resample trials from the original data (500 trials with replacement) and estimate the timescale from the average autocorrelation of resampled data with a direct exponential fit (blue distribution). (c) Average values of timescales estimated by direct fit with non-parametric bootstrap (blue) and parametric bootstrap with bias correction (magenta) deviate from the ground-truth timescale (dashed lines) and the uncertainty intervals (5 and 95 percentiles, error bars) do not contain these ground-truth values for every example. In contrast, the aABC method provides a reliable mean estimate with uncertainty intervals including the ground-truth timescale (orange). Data are generated from an OU process with the given ground-truth timescales and duration $T = 1$ s (500 trials). Bootstrapping and aABC distributions contain 100 samples. For bootstrapping, the error bars are generally smaller than symbol for the average value.



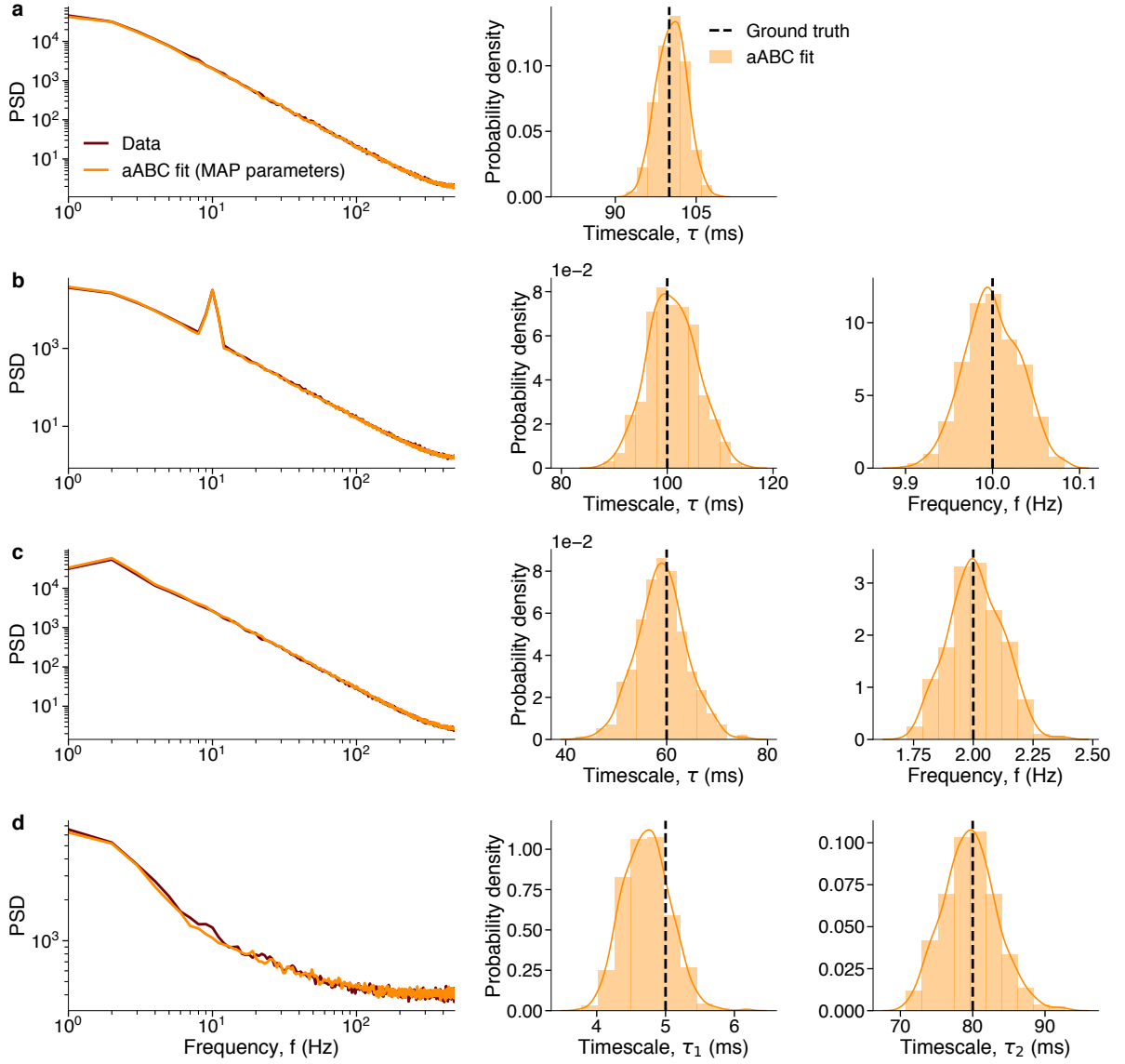
Supplementary Figure 6. Bias in timescales estimated by direct fitting of sample PSD but not in aABC estimates. (a) The shape of sample PSD (brown) deviates from the ground-truth PSD (gray). Knee frequencies estimated by directly fitting the sample PSD with a Lorentzian function (pink) or using the FOOOF toolbox [16] (magenta) are similar and overestimate the ground-truth knee frequency (i.e. underestimate the ground-truth timescale). FOOOF estimates the timescale by fitting the shape of $\log(\text{PSD}(f))$ with the function $b - \log(k + f^\chi)$, where f is the frequency and b , k and χ are free parameters. For an exponential decay function $\chi = 2$, but FOOOF allows for $\chi \neq 2$. The sample PSD is fitted between 1 Hz and 100 Hz frequencies. (b) Timescales estimated in the frequency domain strongly depend on the fitted frequency range and can overestimate, underestimate or produce accurate results depending on the selected frequency range. Distribution of point estimates for the timescales estimated with the FOOOF fit of PSD for 100 independent datasets of the OU process. For each dataset, we averaged the PSD over 500 trials with 1 s duration and the sampling frequency of 1000 Hz. The PSDs are computed using a Hamming window applied to each trial. FOOOF is fitted on the average PSD for each dataset over the frequency ranges of [1, 100] Hz, [1, 200] Hz and [1, 400] Hz from left to right. (c) The aABC method estimates the correct timescales (orange posterior distributions) independent of the selected frequency range. Data are the same as in a and the frequency ranges for fitting are the same as b. The direct-fit estimates (magenta vertical lines) are computed using FOOOF.



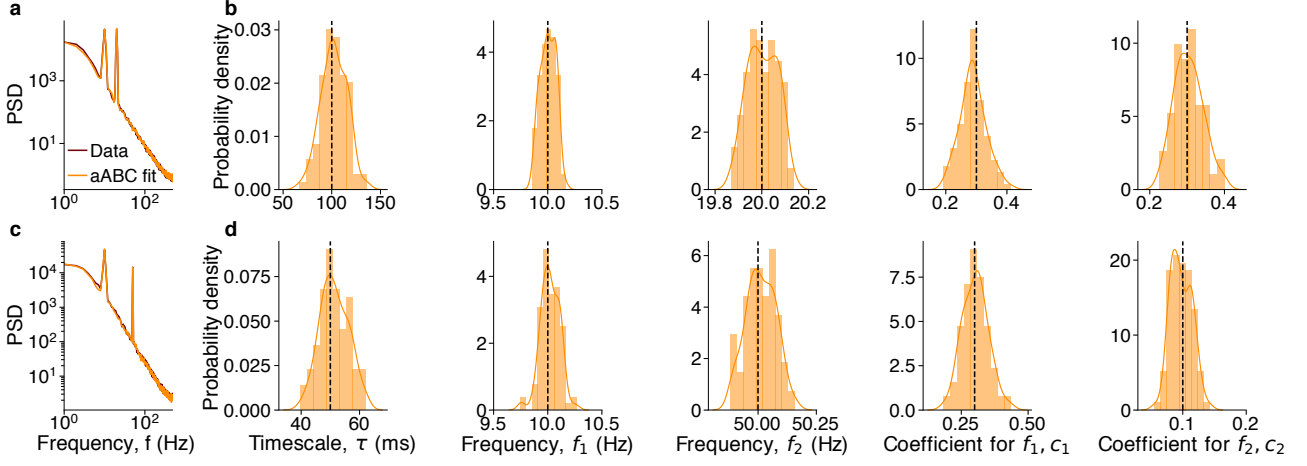
Supplementary Figure 7. Impact of stochasticity on the shape of sample autocorrelation. The shape of sample autocorrelation is slightly different across realizations of the same generative process due to noise in the data. Each trace is the average autocorrelation of 500 trials with $T = 1$ s generated from an OU process with $\tau = 20$ ms.



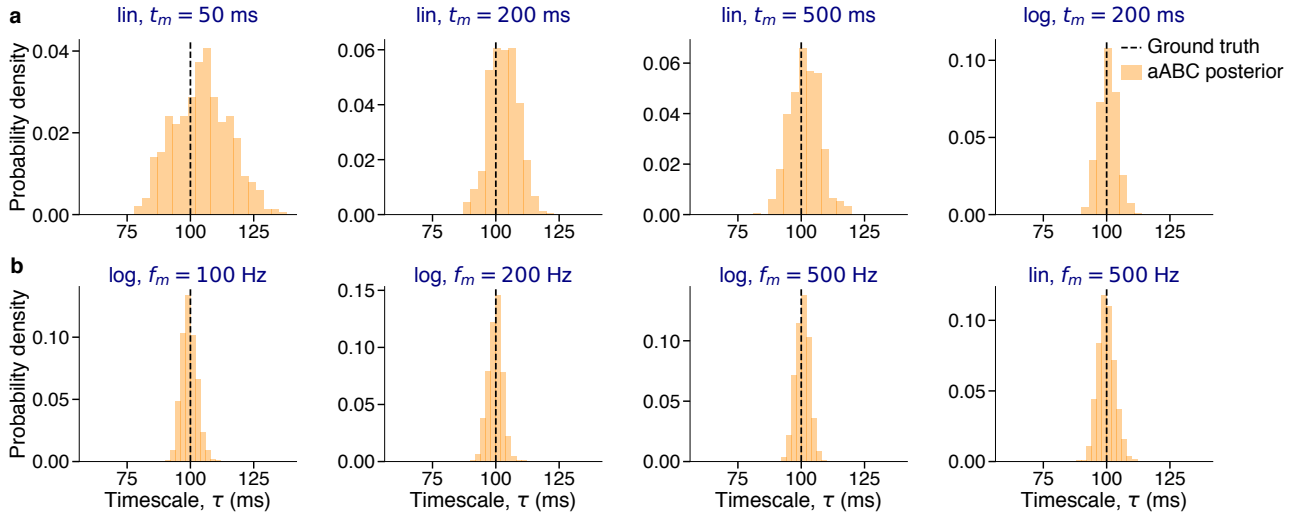
Supplementary Figure 8. Dependence of variance of posterior distributions estimated with aABC on the signal-to-noise ratio. Variance of posterior distributions captures the estimation uncertainty. Increasing the number of trials in observed data reduces the noise in sample autocorrelation (**left**) and the estimation uncertainty (narrower posterior distribution) (**right**). Estimated τ : mean $\pm$ std. The data was generated from an OU process with $\tau = 20$ ms and consisted of trials with $T = 1$ s.



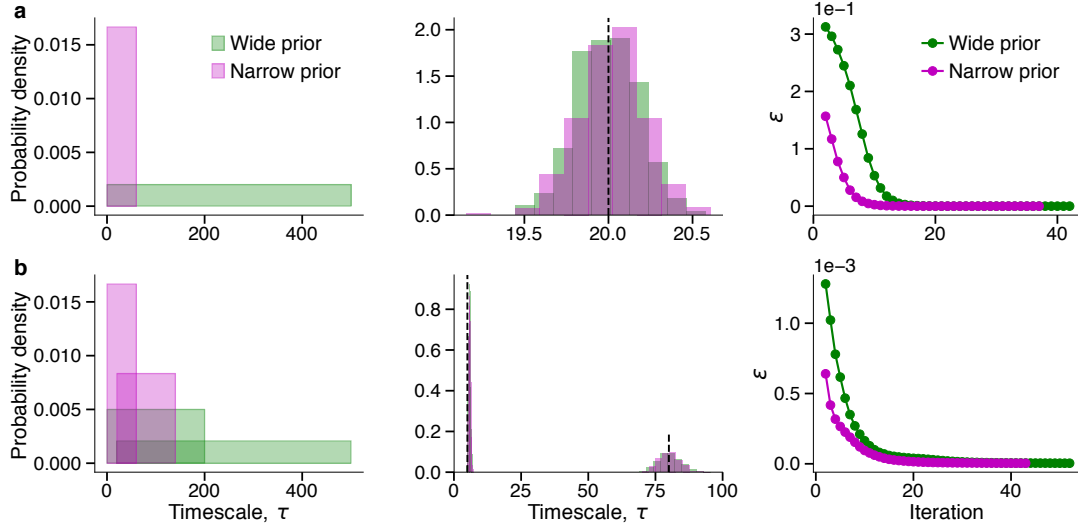
Supplementary Figure 9. Using PSD as the summary statistic in the aABC algorithm. (a) Data are generated from an OU process with the timescale $\tau = 100$ ms. **Left:** The shape of the data PSD (brown) is accurately reproduced by the PSD of synthetic data from the generative model with the MAP estimate parameters (orange). **Right:** The marginal posterior distributions (histograms overlaid with Gaussian kernel smoothing) recover the ground-truth parameters. (b) same as a for data from a linear mixture of an OU process with the timescale $\tau = 100$ ms and an oscillation with frequency $f = 10$ Hz. (c) Same as b with $\tau = 100$ ms and $f = 2$ Hz. The slow oscillation does not manifest in any clear peak in PSD due to short duration of trials ($T = 1$ s) and the low frequency resolution. However, aABC algorithm can still uncover the oscillatory component with the correct parameters. (d) same as a for data from an inhomogeneous Poisson process with two timescales $\tau_1 = 5$ ms and $\tau_2 = 80$ ms.



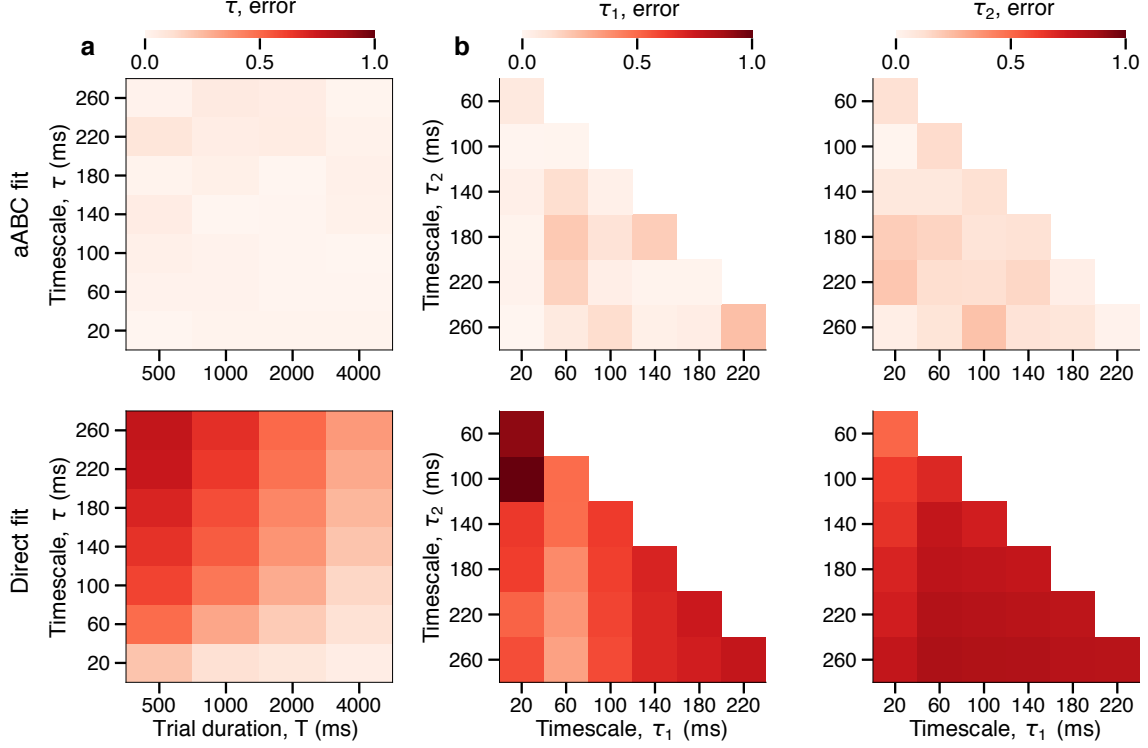
Supplementary Figure 10. Accuracy of aABC estimates in the presence of multiple oscillatory components. (a-b) Data are generated from a linear mixture of an OU process with the timescale $\tau = 100$ ms and two oscillations with frequencies $f_1 = 10$ Hz and $f_2 = 20$ Hz with coefficients $c_1 = c_2 = 0.3$. (a) The shape of the data PSD (brown) is accurately reproduced by the PSD of synthetic data from the generative model with the MAP estimate parameters (orange). (b) The marginal posterior distributions (histograms overlaid with Gaussian kernel smoothing) recover the ground-truth parameters (vertical dashed lines). (c-d) same as a-b with $\tau = 50$ ms, $f_1 = 10$ Hz, $f_2 = 50$ Hz, $c_1 = 0.3$ and $c_2 = 0.1$.



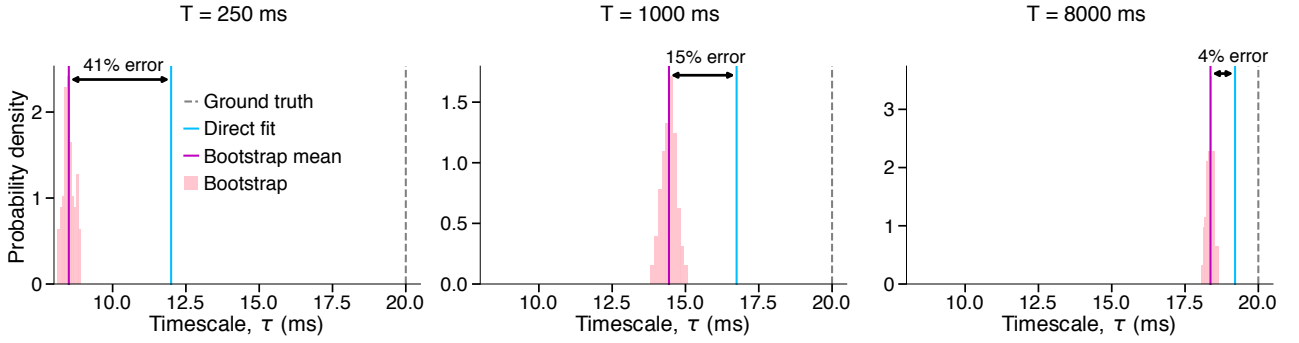
Supplementary Figure 11. Recovering the ground-truth timescales with posterior distributions approximated by the aABC method independent of the selected summary statistic and fitting range. Data are generated from an OU process with the timescale $\tau = 100$ ms. (a) The aABC algorithm fitted the data autocorrelation up to the time-lag t_m (indicated in the figure title) using distances computed in linear (lin) or logarithmic (log) scale. (b) The aABC algorithm fitted the data PSD from $f = 1$ Hz up to the frequency f_m (indicated in the figure title) using distances computed in linear (lin) or logarithmic (log) scale.



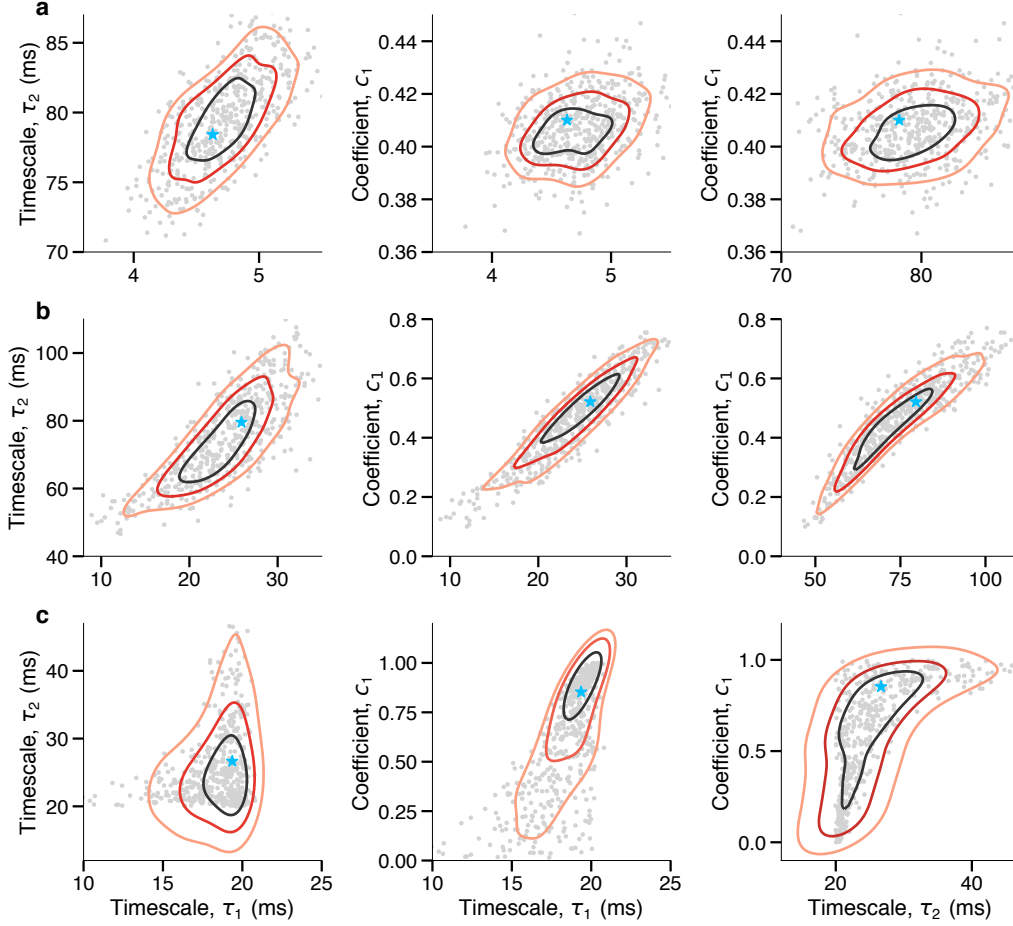
Supplementary Figure 12. Impact of the width of prior distributions for generative model parameters on the shape of posterior distributions and the speed of aABC convergence. (a) Wide and narrow prior distributions (left) give rise to similar posterior distributions (middle), but aABC fit with a narrower prior converges in fewer iterations (right). Data are generated from an OU process with the timescale $\tau = 20$ ms and fitted with aABC algorithm and PSD as a summary statistic using two different prior distributions: narrow prior $\tau : U[0, 60]$ and wide prior $\tau : U[0, 500]$ ms, where $U[\cdot, \cdot]$ denotes a uniform distribution. The vertical dashed line indicates the ground-truth timescale. Error thresholds (ε) are plotted starting from the second iteration. Initial error threshold for all fits was set to 1. (b) same as a for data generated from an inhomogeneous Poisson process with two timescales $\tau_1 = 5$ ms and $\tau_2 = 80$ ms and prior distributions: narrow prior $\tau_1 : U[0, 60]$ ms, $\tau_2 : U[20, 140]$ ms; wide prior $\tau_1 : U[0, 200]$ ms, $\tau_2 : U[20, 500]$ ms.



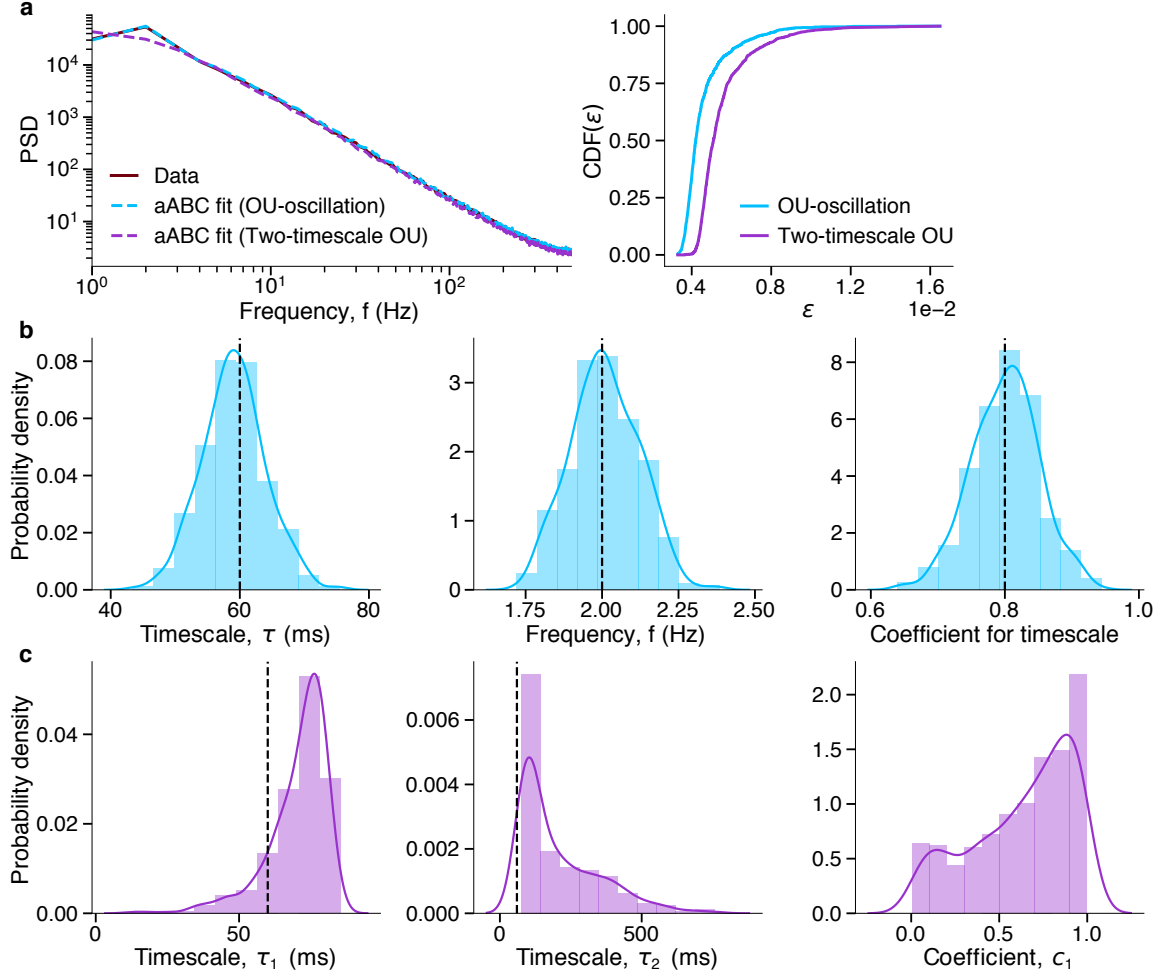
Supplementary Figure 13. Comparison of goodness of fit for the aABC and direct fitting. (a) The estimation error of the MAP estimates from the aABC fit is always small (upper panel), whereas the estimation error of the direct fit depends on the trial duration relative to the ground-truth timescale (lower panel). Data for each fit are generated from an OU process with the given timescales τ and the trial duration T (500 trials). Estimates of direct fits are computed from fitting the autocorrelation shape with an exponential decay function. Errors are computed as $|\text{ground-truth timescale} - \text{estimated timescale}| / (\text{ground-truth timescale})$. (b) same as a, for data generated from two-timescale OU processes with the given τ_1 and τ_2 timescales, coefficients $c_1 = c_2 = 0.5$ and trial duration of $T = 1000$ ms. MAP estimates for both timescales from the joint posterior distribution are always more accurate than direct fitting with the double-exponential function. Here, the relationship between the values of two timescales and accuracy is non-monotonous. In addition, the aABC method returns a full posterior for each estimate (not only the MAP estimate) and the ground-truth timescales are within the bounds of posterior.



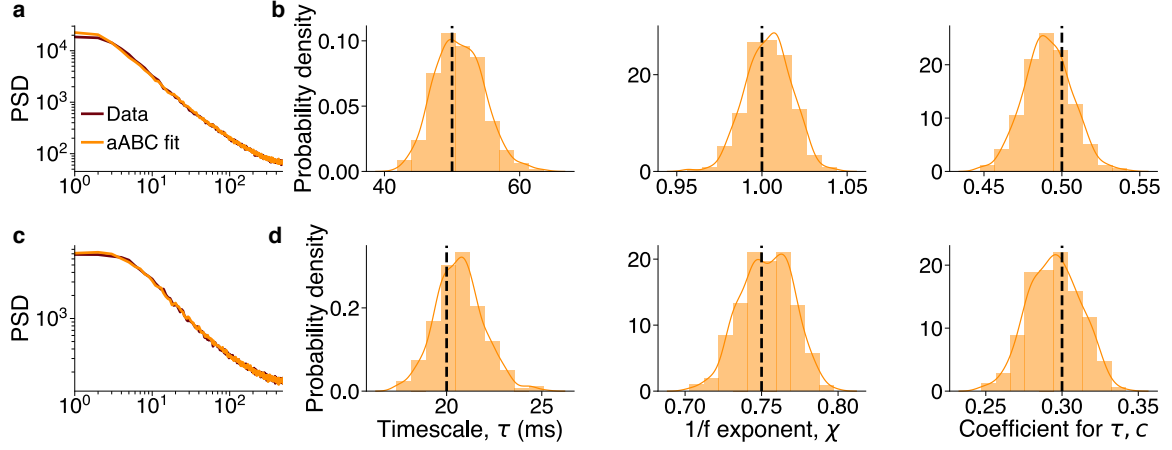
Supplementary Figure 14. Evaluating the quality of direct fit using abcTau package pre-processing functionality. We use the parametric bootstrapping method to evaluate the quality of direct fit. We generate multiple synthetic datasets from a generative model with parameters estimated by the direct fit and estimate the timescale from each of these datasets again by direct fitting. If the error between the mean of bootstrapping estimates and original direct fit is small enough (based on a user-defined tolerance) the direct fit estimate can be used. Since the bootstrapping error can be smaller than the true error (error between the ground-truth timescale and the direct fit estimate), users should consider setting a stricter tolerance than required. Data in each panel are generated from an OU process with timescale $\tau = 20$ ms and the indicated trial duration T (500 trials). Increasing the trial duration leads to smaller errors for the direct fit estimates. Errors (black arrows) are computed as $|\text{direct-fit estimate} - \text{mean}(\text{bootstrapping distribution})|/(\text{direct-fit estimate})$.



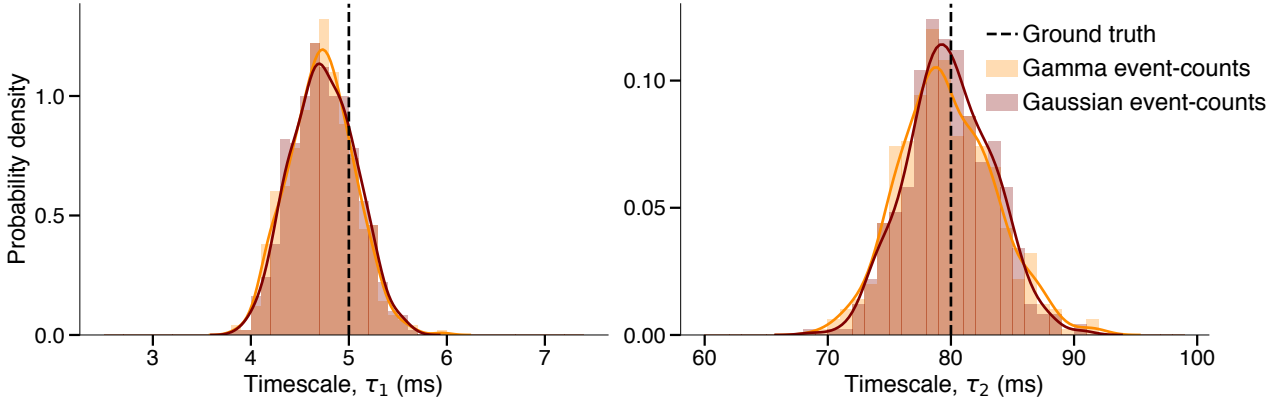
Supplementary Figure 15. Evaluating the relation between parameters in the joint posterior distributions from the aABC method. (a-c) Bivariate marginal distributions obtained from the three-dimensional posterior distribution of parameters from fitting a two-timescale model on different example data (same data as in Fig. 5). Isolines are computed by fitting bivariate Gaussian kernel density on the posterior samples and indicate the parameter combinations with equal probability in the joint posterior (isoline levels are set at $p = 0.75, 0.5, 0.25$ from the inner to outer contours, i.e. for 0.25 isoline 25% of the probability mass will lie within the contour). The blue star shows the MAP estimate from the joint posterior distribution and the gray dots show the samples of the posterior. (a) When data has two clear distinct timescales ($\tau_1 = 5$ ms, $\tau_2 = 80$ ms) the joint marginals have a clear peak (black isoline with $p = 0.75$) around the MAP estimate and parameters are more independent from each other (i.e. circular shape of bivariate distributions). (b) When the timescales are closer to each other ($\tau_1 = 20$ ms, $\tau_2 = 80$ ms) and the distinction between the timescales is less clear in the autocorrelation shape (Fig. 5c), the parameters become more correlated in the posterior. (c) When data has only one timescale ($\tau = 20$ ms), there is a degeneracy in parameters of the two-timescale model and fit provides different possible solutions: (i) both timescales are close to the ground truth and the coefficient takes a broad range of values with the same probability, indicating that the coefficient is a sloppy parameter, (ii) one of the timescales is away from the ground truth and its coefficient is close to zero, suggesting that this additional timescale is a sloppy parameter. This degeneracy indicates that the model is overparametrized. Note that we enforce $\tau_1 < \tau_2$ which generates asymmetry in the posterior.



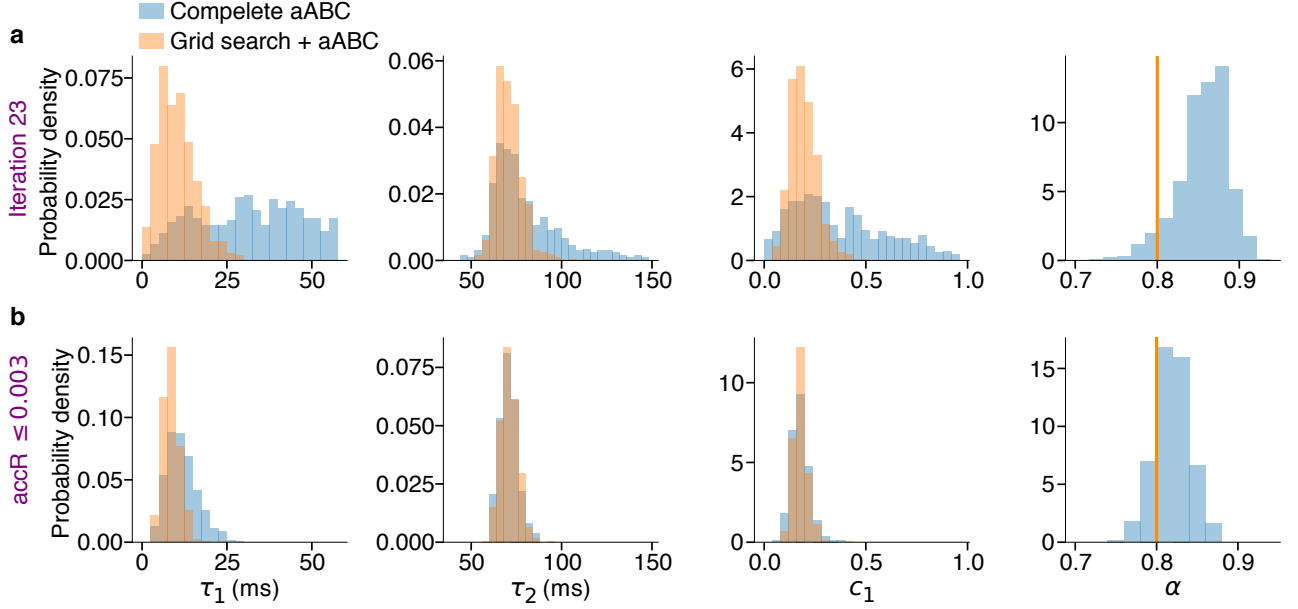
Supplementary Figure 16. Discrimination between periodic (oscillatory) and aperiodic (exponential decay) components using model selection with ABC. (a-c) Data are generated from a linear mixture of an OU process with the timescale $\tau = 60$ ms and an oscillation with frequency $f = 2$ Hz (same as Supplementary Figure 9c). Using the ABC model comparison method, we tested whether the shape of the PSD from these data can be equally well described with a two-timescales OU process without any oscillatory components. (a) The data PSD is fitted with two models: 1) a linear mixture of an OU process and oscillation (blue), 2) a two-timescale OU process (purple) (left). Since cumulative distribution of distances for the first model is larger than for the second model for all ε , the model with the linear mixture of an OU process and oscillation is selected (right). (b) The marginal posterior distributions (histograms overlaid with Gaussian kernel smoothing) for the linear mixture of an OU process and oscillation. Vertical lines indicate the ground-truth values. (c) The marginal posterior distributions (histograms overlaid with Gaussian kernel smoothing) for the two-timescale OU process. Vertical lines indicate the ground-truth value of the single ground-truth timescale.



Supplementary Figure 17. Estimating timescales with aABC in the presence of background processes. (a-b) Data are generated from a linear mixture of an OU process with the timescale $\tau = 50$ ms (coefficient $c = 0.5$) and random time-series generated from a $1/f$ PSD shape with exponent $\chi = 1$ over the frequency range of $[1, 500]$ Hz (corresponding to the time-domain signals with $T = 1$ s duration). (a) The shape of the data PSD (brown) is accurately reproduced by the PSD of synthetic data from the fitted generative model with the MAP estimate parameters (orange). The generative model is the same as for the original data (i.e. a linear mixture of an OU process and random time-series generated from a $1/f$ PSD shape). (b) The marginal posterior distributions (histograms overlaid with Gaussian kernel smoothing) recover the ground-truth parameters (vertical dashed lines). (c-d) same as a-b with $\tau = 20$ ms, $\chi = 0.75$, $c = 0.3$.



Supplementary Figure 18. Similar aABC fits using doubly stochastic generative models with the Gaussian or gamma distributions of event-count. We fitted the inhomogeneous Poisson process example from Fig. 1c using aABC with generative models which had a Gaussian or gamma event-count distributions with $\alpha = 1$. Both generative models recover the ground-truth timescales and produce posterior distributions that are not significantly different (Wilcoxon rank-sum test: $P_{\tau_1} = 0.23$, $P_{\tau_2} = 0.37$).



Supplementary Figure 19. Estimating the parameter α of the doubly stochastic generative model with aABC and with the grid search. We fitted the neural data autocorrelation in Fig. 6 considering α as an additional parameter of the generative model estimated with aABC (complete aABC). We compared the results of complete aABC with first estimating α with a grid search and then fitting the rest of parameters with aABC (grid search + aABC). **(a)** Starting from the same error threshold $\varepsilon = 1$, after the same number of iterations (23), the complete aABC has a larger variance of marginal posterior distributions than the grid search + aABC. This result indicates that the grid-search method reaches narrower posteriors in fewer iterations. Moreover, for the complete aABC, the posterior of α is relatively narrow, while posteriors of all other parameters are wider at iteration 23. This observation shows that the complete aABC fits α first and almost independently from the other parameters of the generative model. **(b)** After running both methods until they reach $accR \leq 0.003$, MAP estimates with complete aABC converge toward the estimations from the grid search + aABC.