

Tuning Strategy

The procedure to obtain efficient convergence of the posterior samples by tuning the number of iterations in the MCMC algorithm.

To obtain posterior samples with reasonable speed, the length of the burn-in period, thinning rate, and effective iteration number in CMBI might be needed to be tuned as follows (Gelman et al., 2013). These values are located in the section named `Iteration numbers` in

`'MBI_single_cell_main.R'`, `'MBI_multiple_cells_main.R'`, and

`'MBI_multiple_cells_same_n_main.R'`.

Step1. Adjust `burn`, which represents the number of iterations which are discarded to make the left Gibbs samples independent from the initial value. Its default value is 10^3 in our code.

The value of `burn` can be set to a smaller or larger value than the default value, 10^3 , if the drift from the initial value of the parameter in the trace plot is finished before or after 10^3 iterations, respectively.

Step2. Adjust `jump`, which represents the reciprocal of the thinning rate. Its default value is 10, which means that, every 10 samples, one sample is selected as a posterior sample and the others are discarded. The value of `jump` can be set to a smaller or larger value than the default value, 10, if the autocorrelation of the remaining samples drops to zero within 10 lags or beyond 10 lags, respectively.

Step3. Adjust `effnum`, which represents the number of posterior samples that are given as outputs of the codes. Its default value is 10^3 . The value of `effnum` can set to be a smaller value than the default value, 10^3 , if the histogram of 10^3 posterior samples is the same to that of $< 10^3$ posterior samples. On the other hand, the value can set to be a larger value if the histogram of 10^3 posterior samples is different with that of $> 10^3$ posterior samples.

The procedure to obtain efficient convergence of the posterior samples by tuning the variances of the proposal distributions for the Metropolis-Hastings algorithm.

As well as tuning the iteration number, the variance of the proposal distributions in the section named `Proposal variances` might be needed to be tuned. Specifically, users need to adjust the variance to achieve the reasonable acceptance rate between 0.2 and 0.5 (Gelman et al., 2013). For this, users need to increase the variance if the acceptance rate is > 0.5 . On the other hand, if the acceptance rate is < 0.2 , users need to decrease the variance. Users can adjust the variance by quickly checking the acceptance rate with the current variance through running only few iterations ($\sim 10^2$) without the burn-in period and thinning (i.e., `burn=0` and `jump=1`).

In ‘`MBI_single_cell_main.R`’, there are three variables `AR_death`, `AR_n`, and `AR_tr` representing the acceptance rates of the posterior samples of λ_d, n , and t_r , respectively. After checking these variables, users may need to adjust `prop_var_death`, `prop_var_n`, and `prop_var_tr` representing the variances of the normal proposal distributions for λ_d, n , and t_r , respectively. Note that there is no proposal variance for λ_b because its posterior samples are directly sampled from the conditional posterior distribution without using the Metropolis-Hastings algorithm.

In ‘`MBI_multiple_cells_main.R`’, there are two variables `AR_hyper` and `AR_param` representing the acceptance rates of the posteriors samples of the hyperparameters, and that of the parameter sets of the D single cells, respectively. `AR_hyper` has 8 elements that are the acceptance rates of the 8 hyperparameters $(\alpha_{\lambda_b}, \beta_{\lambda_b}, \alpha_{\lambda_d}, \beta_{\lambda_d}, \alpha_n, \beta_n, \alpha_{t_r}, \beta_{t_r})$. `AR_param` is $D \times 4$ matrix. The four elements in the j -th row are the acceptance rate of $\lambda_b^{(j)}, \lambda_d^{(j)}, n^{(j)}$, and $t_r^{(j)}$ of the j -th cell. After checking these acceptance rate, users may need to adjust the proposal variances, `hyper_prop_var` and `prop_var`. `hyper_prop_var` has 8 elements

that are the proposal variances of the 8 hyperparameters, and the j -th row of `prop_var` has 4 elements that are the proposal variances of $\lambda_b^{(j)}, \lambda_d^{(j)}, n^{(j)}$, and $t_r^{(j)}$, for $j = 1, \dots, D$. We let the proposal variances of $\lambda_b^{(i)}, \lambda_d^{(i)}, n^{(i)}$, and $t_r^{(i)}$ be the same to those of $\lambda_b^{(j)}, \lambda_d^{(j)}, n^{(j)}$, and $t_r^{(j)}$ for arbitrary i and j .

References

Gelman, A., Carlin, J.B., Stern, H.S., Dunson, D.B., Vehtari, A., and Rubin, D.B. (2013). Bayesian data analysis (CRC press).