A parallel algorithm for fitting the parameters of a stochastic model in systems biology

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In recent years, stochastic models have been used intensively in systems biology to describe the biochemical network dynamics. Nevertheless, the problem of fitting the unknown parameters in a stochastic model to experimental data remains challenging. The discrepancy between the data and the model can be captured in the likelihood function, which acts as the 'distance' to be minimized by the parameter set. Many models, however, can have the identifiability problem or confounded parameters, and the likelihood function can be multimodal [1]. An optimization scheme, therefore, has to start from many different initial guesses and the final guess for the parameters demands a large number of likelihood calculations. For complicated models, this can be time-consuming, especially if implemented as a serial algorithm in which only one optimization iteration can run at a time.

In this work, we parallelize the parameter fitting process. Independent optimization iterations can run from different initial guesses at the same time, therefore reducing the time cost. An inhibitory model in Escherichia coli [2] is used in the numerical experiment, where five unknown parameters need to be fitted to the observed protein counts at various time points. We investigate the performance of the parallel code with respect to the number of cores, and the efficiency of the resulting parameter set in recreating the frequencies observed in the experimental data. This work can serve as a more general framework for parameter fitting in demanding problems in systems biology.

References

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