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Supplementary Information

Self-learning Entropic Population Annealing for Interpretable Materials Design

Jiawen Li[1], Jinzhe Zhang[1], Ryo Tamura*[1,2,3,4], and Koji Tsuda*[1,3,4]

1 Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, Chiba 277-8561, Japan

2 International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

3 Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

4 RIKEN Center for Advanced Intelligence Project, 1-4-1 Nihonbashi, Chuo-ku, Tokyo 103-0027, Japan

Dependency on number of iterations and inverse temperatures

In SLEPA and EPA, some hyperparameters are existed. In this supplementary note, we address dependencies on number of iterations τ and the maximum inverse temperature $\beta_{\max}$ when the number of observations is fixed. If τ is changed, the number of particles M should be changed to fix the number of observations. Figure S1 shows the Hellinger distance of the residue distribution to the ground truth distribution depending on τ, M, and $\beta_{\max}$. First, for our problems, $\beta_{\max} = 10$ is the best choice for the small percentile cases. If SLEPA is used, when the number of observations is small (i.e., 1000 and 4000), the value of τ should be increased instead of M to obtain better results. When the number of observations is large enough as 20000, the dependency on τ and M is not observed for SLEPA. On the other hand, for EPA, the opposite situation is preferred, that is, M should be increased than τ. Thus, we confirm that $\tau = 20$ used in the main text shows relatively better results for both SLEPA and EPA. Furthermore, if the any values of τ and M are used, the results by SLEPA are better than those by EPA for small percentile cases when $\beta_{\max} = 10$. Note that the optimum value of $\beta_{\max}$ strongly depends on the problem, in particular the energy value, $e(\mathbf{x})$.

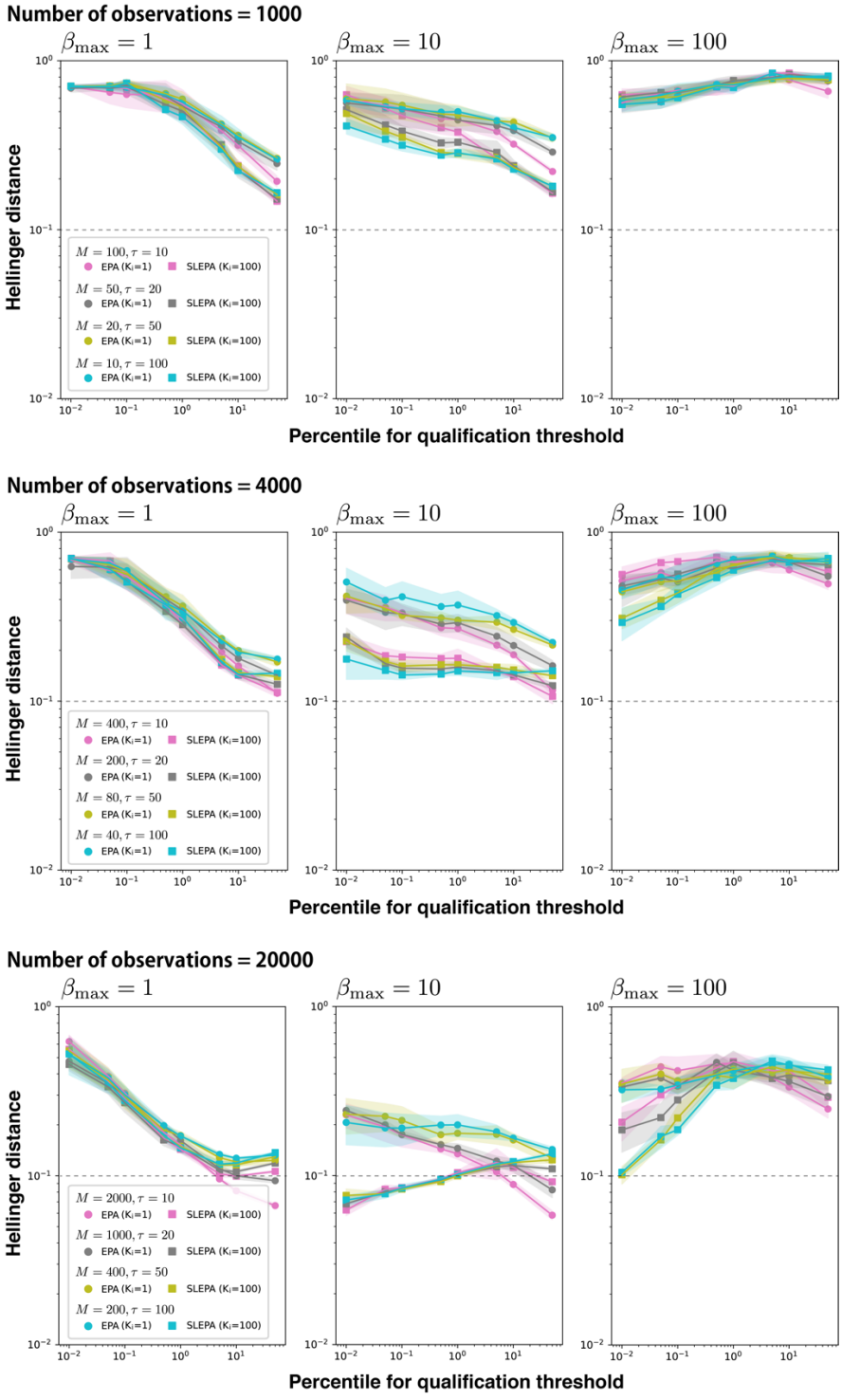

Fig. S1. Hellinger distance of the residue distribution to the ground truth distribution against the qualification threshold depending on the number of observations. Dependencies on numbers of particles M and iterations τ and $\beta_{\max}$ are summarized when $\beta_{\min}$ is fixed as 0.