

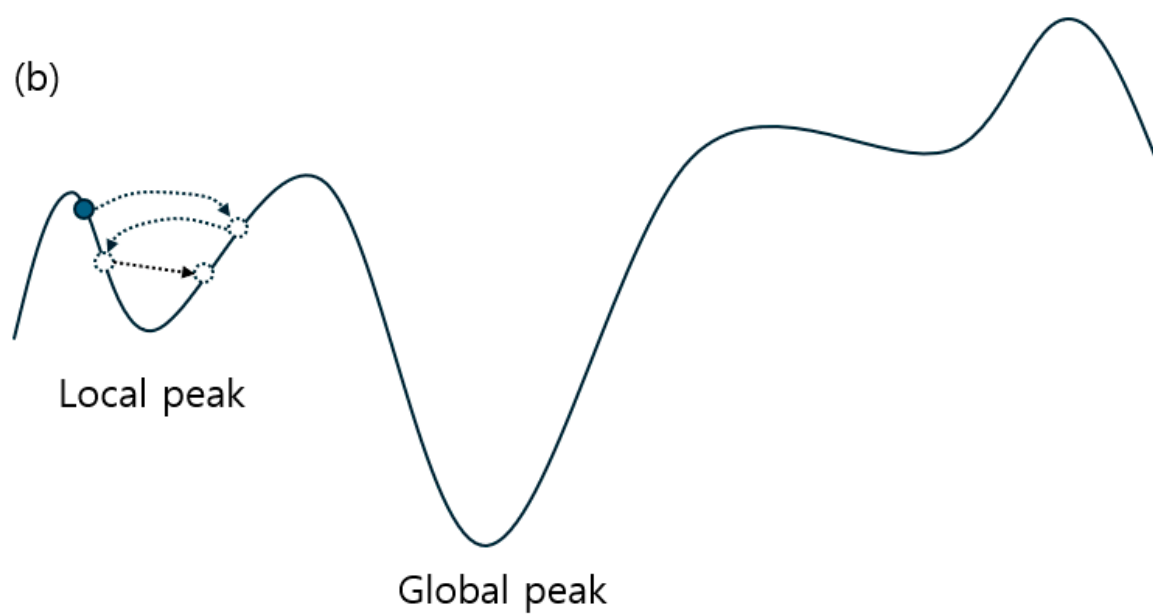
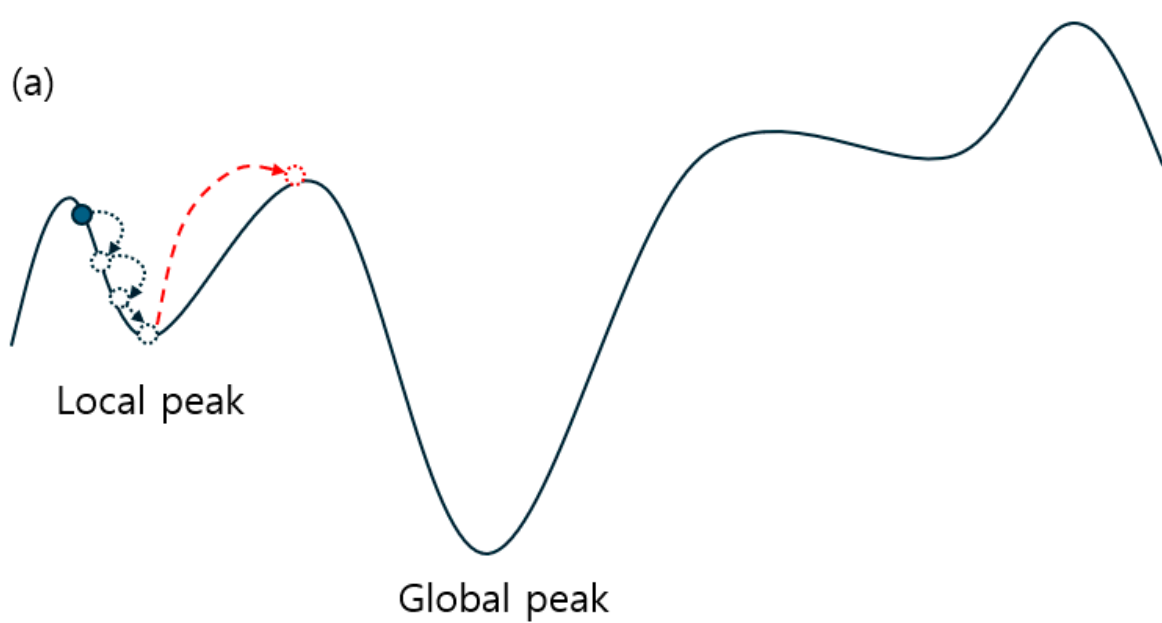
Supplementary File S1. The CASOH sampling explanations.

Figure S(a) illustrates a single Metropolis-Hastings sample with a small step size, where the initial position is near a local peak, assuming two minimum peaks in the regression task. In this scenario, the system's local peak is easily identified. However, escaping the local peak to reach the global peak is challenging due to the small step size.

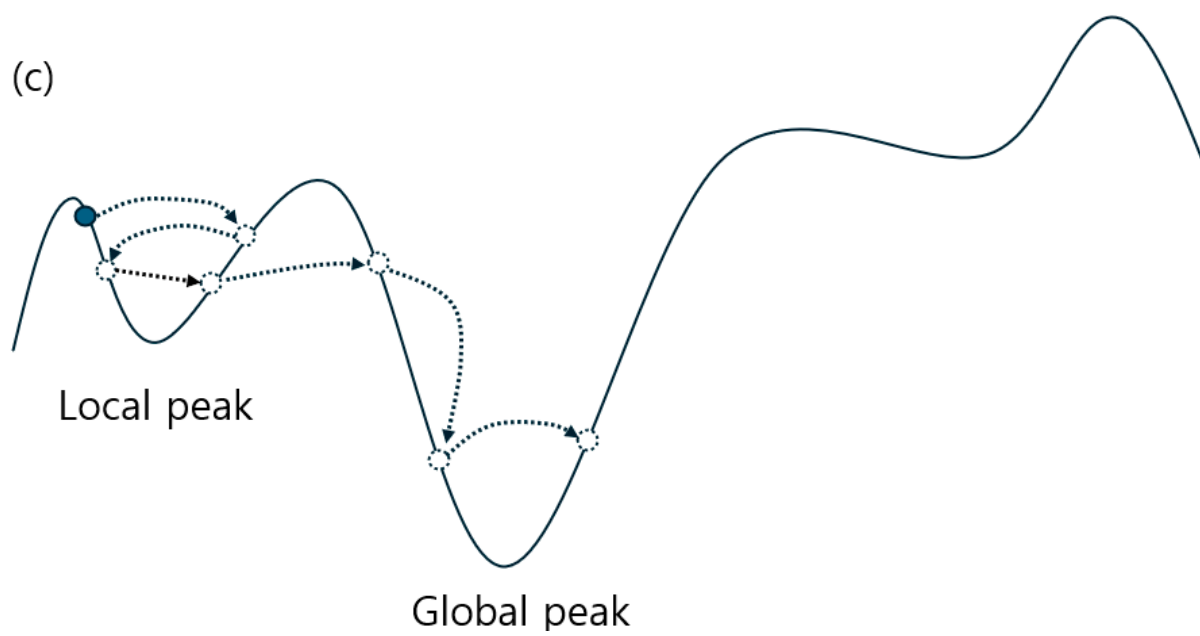
In Figure S(b), increasing the step size allows for a better peak can be found. Yet, the sample often remains trapped in the local peak. In some cases, worse results may emerge compared to Figure S(a). Fortunately, as the number of iterations increases (see Figure S(d)), better results can be achieved compared to Figure S(a). Nonetheless, the global peak remains elusive, and the results continue to fluctuate. If the step size increases further, the results worsen, and the system fails to converge, as shown in Figure S(c).

These observations suggest that the outcomes strongly depend on the chosen step size, leading to significant computational costs due to trial and error. To address this limitation, we propose a combined sampling algorithm where the Metropolis-Hastings sample is integrated with a random sample (see Figure S(e)).

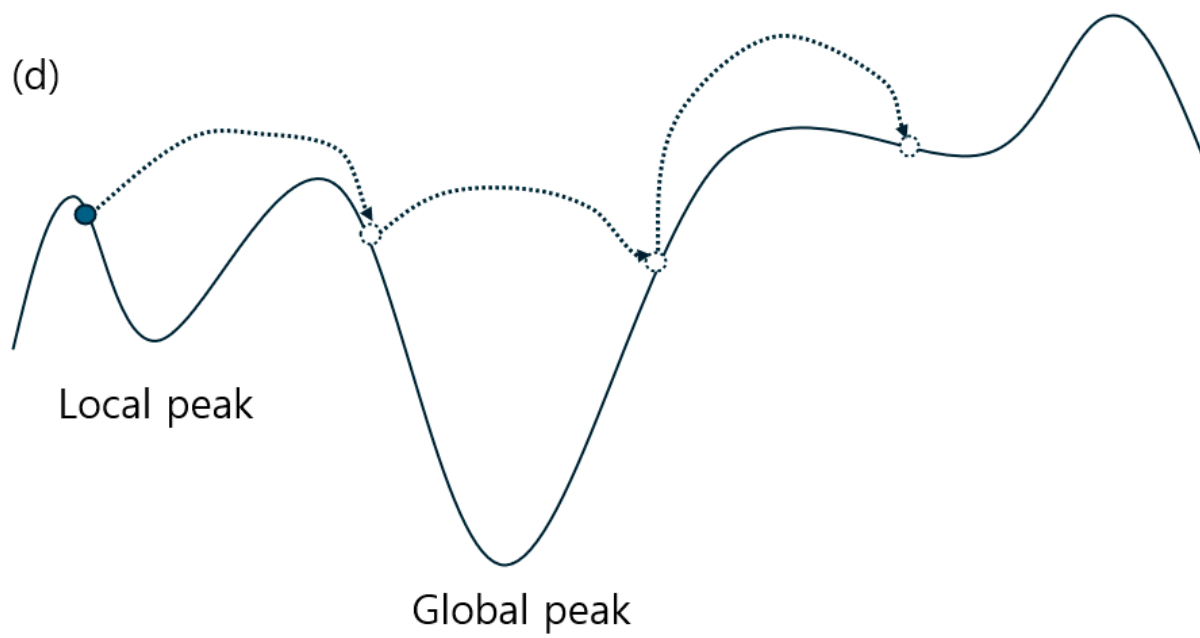
This algorithm introduces a random number to determine whether a sample is accepted, leveraging an acceptance probability. By employing this acceptance probability, the algorithm allows trapped samples to escape local peaks and progressively move toward the global peak. It consistently identifies better system states. The acceptance probability serves as a parameter linking the Metropolis-Hastings sample with the random sample. Consequently, this proposed combined sampling approach significantly increases the likelihood of locating the global peak.



(c)



(d)



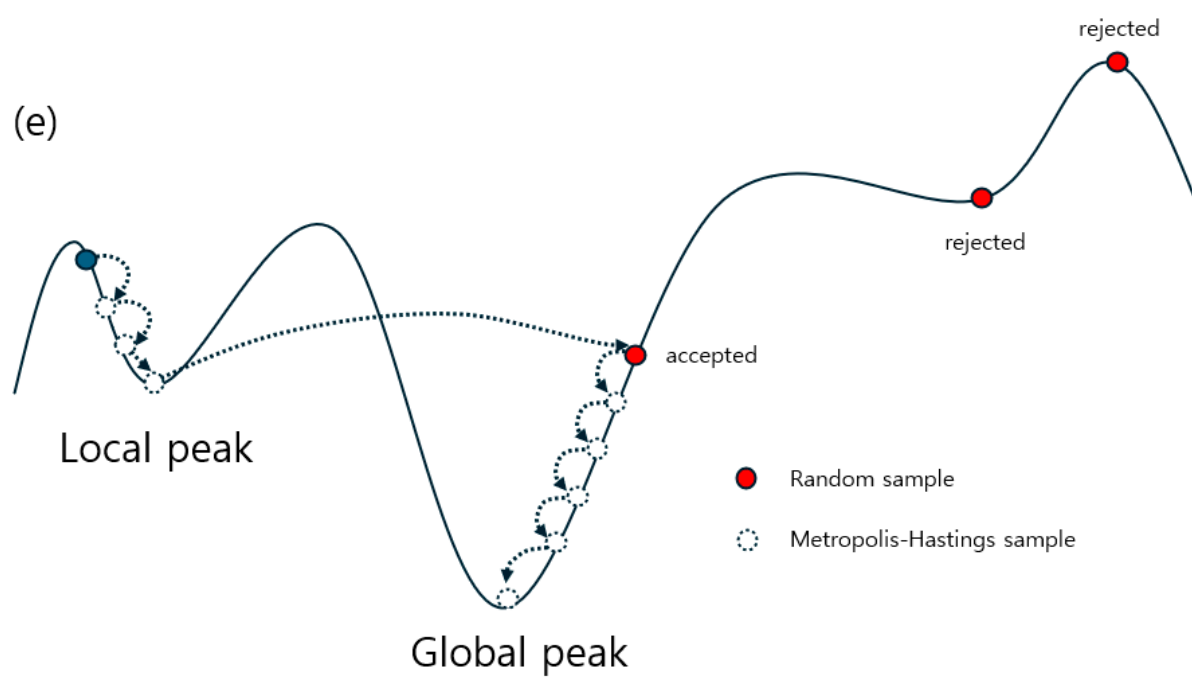


Figure S1. An explanation for the CASOH sampling algorithm