

Parallel Tempering Pseudocode

Let S be an arbitrary state space with an associated cost function $\omega: S \rightarrow \mathbb{R}$ and a set of transitions $E \subseteq S \times S$. Let $V = \{\omega(s): s \in S\}$. Then $G = (V, E)$ is a network of weighted states and transitions.

Let T be a finite subset of real numbers (representing the "energy" of a replica).

Let L be a natural number (representing the number of independent transitions prior to a "neighbor swap").

Let R be an ordering of $\{1, \dots, |T| - 1\}$ (representing an ordering of the replicas).

Let $\delta_1 = \delta_2 = \dots = v$, where v is a uniform randomly selected element of V .

loop an arbitrary number of times

for all $i \in \{1, \dots, |T|\}$ **do**

loop L times

 Let δ' be a uniform randomly chosen neighbor of δ_i .

 Let $p = \min\{1, \exp[(1/T_i)(\omega(\delta_i) - \omega(\delta'))]\}$

 Let $\delta_i = \delta'$ with probability p .

end loop

end for

for all $i \in R$ **do**

 Let $p = \min\{1, \exp[(1/T_i - 1/T_{i+1})(\omega(\delta_i) - \omega(\delta_{i+1}))]\}$

 Swap δ_i, δ_{i+1} with probability p .

end for

end loop