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Katsunori Kubo, ASRC, JAEA

Importance sampling

Procedure to make samples

We want to make a sequence of states $\{x_i\}$ ($i = 1, 2, \cdots$) such that the number of i with $x_i = x$ is proportional to distribution $P(x)$. For this purpose, the following procedure is known:

1. When the state is x, we choose the state y as the next candidate with probability $S(x \to y)$. The followings are assumed:
   - $\sum_y S(x \to y) = 1$.
   - $S(x \to y) = S(y \to x)$.
   - All the states are connected by non-zero S (It is not necessary to be directly connected).
2. When y is selected as the next candidate, we update the state to y with probability $w(x \to y)$. We assume

$$P(x)w(x \to y) = P(y)w(y \to x).$$

   This condition is known as the detailed balance.

To fulfill this condition, for example, we can take

$$w(x \to y) = \begin{cases} P(y)/P(x) & \text{if } P(y) < P(x) \\ 1 & \text{otherwise} \end{cases}.$$

This is known as the Metropolis method.

Proof on the distribution of the samples

We prepare many systems and suppose that N_x systems are in state x. In the next step, by using the detailed balance, the change of the number of the systems with state x is

$$\begin{aligned}
&\sum_{y\neq x} N_y S(y \to x) w(y \to x) - \sum_{y\neq x} N_x S(x \to y) w(x \to y) \\
&= \sum_{y\neq x} \left[N_y S(x \to y) \frac{P(x)}{P(y)} w(x \to y) - N_x S(x \to y) w(x \to y) \right] \\
&= \sum_{y\neq x} N_y S(x \to y) w(x \to y) \left[\frac{P(x)}{P(y)} - \frac{N_x}{N_y} \right].
\end{aligned}$$

When $P(x)/P(y) > N_x/N_y$, N_x is increased from the contributions of the systems with state y. When $P(x)/P(y) < N_x/N_y$, N_x is decreased from the contributions of the systems with state y. By repeating this procedure, for all the states y with non-zero $S(x \to y) = S(y \to x)$, the relation $N_y/N_x = P(y)/P(x)$ will be reached. All the states x obey the distribution $P(x)$ when all the states are connected by non-zero S.
To consider many systems is equivalent to make many states in a system.

References

[1] K. Binder and D. W. Heermann "Monte Carlo Simulation in Statistical Physics" 5th ed. (Springer, 2010) p. 17.