Equations

Consider a system of N points, each with a dimensionality d. Our target distribution ($\mathbf{P}$, assuming it is normalized) is defined in terms of some function ($\mathbf{W}$) which is somehow related to the Potential Energy ($\mathbf{V}$).

$$\begin{aligned}
\mathbf{P}(\mathbf{x}) &:= e^{-\mathbf{W}(\mathbf{x})} \\
\mathbf{W}(\mathbf{x}) &= -\ln\{\mathbf{P}(\mathbf{x})\} \\
\mathbf{x}_i &= (x_i^1, \ldots, x_i^d) \\
\text{N points} &= \sum_{i=1}^{N} \mathbf{x}_i
\end{aligned} \tag{1}$$

To generate $\mathbf{P}(\mathbf{x})$, such that that distance between points follows a regular grid (a quasi-crystal) we introduce a quasi Lennard-Jones Pair-Wise Potential, $\mathbf{U}$.

$$\begin{aligned}
\mathbf{U}_{ij}(\mathbf{x}_i, \mathbf{x}_j) &:= 4\epsilon \left\{ \left[\frac{\sigma_i(\mathbf{x}_i) + \sigma_j(\mathbf{x}_j)}{|\mathbf{x}_{ij}|} \right]^{12} - \left[\frac{\sigma_i(\mathbf{x}_i) + \sigma_j(\mathbf{x}_j)}{|\mathbf{x}_{ij}|} \right]^{6} \right\} \\
|\mathbf{x}_{ij}| &= \sum (\mathbf{x}_i - \mathbf{x}_j)^2
\end{aligned} \tag{2}$$

ϵ is a parameter essentially playing the role of temperature in our system.

The function σ returns a constant, and is essentially the distance between points in the regular grid representing $\mathbf{P}(\mathbf{x})$.

$$\sigma_i = \sigma(\mathbf{x}_i) := c \cdot [N \cdot P(\mathbf{x}_i)]^{-1/d} \tag{3}$$

Sigma is given scaling with respect to the total number of points and their dimensionality respectively. The constant c should be on the order of 1.

To generate $\mathbf{P}(\mathbf{x})$ a Metropolis Monte Carlo algorithm is implemented with an acceptance criteria in terms of a uniformly distributed random number $0 < t < 1$.

$$t > \exp\{\beta \Delta \mathcal{U}\} \tag{4}$$

where,

$$\mathcal{U} = \sum_{i=1}^{N} \mathbf{V}(\mathbf{x}_i) + \sum_{i,j} \mathbf{U}_{ij}(\mathbf{x}_i, \mathbf{x}_j) \tag{5}$$

This is analagous to evaluating

$$\frac{\mathbf{P}(\mathbf{x}_{trial})}{\mathbf{P}(\mathbf{x}_i)} \tag{6}$$

Gaussain Target Distribution

Consider a specific case, where we define a harmonic potential

$$\mathbf{W} := \mathbf{V} = \frac{\mathbf{x}^2}{2} \tag{7}$$

Our definition of $\mathbf{P}(\mathbf{x})$ becomes

$$\mathbf{P}(\mathbf{x}) := (2\pi)^{-d/2}\, e^{-\frac{\mathbf{x}^2}{2}} \tag{8}$$

Where the pre-factor is a normalization constant for the target distribution $\mathbf{P}(\mathbf{x})$.