Structure relaxation using Kernel Ridge Regression

Malthe Kjær Bisbo

April 3, 2018

ML-enhanced Monte Carlo
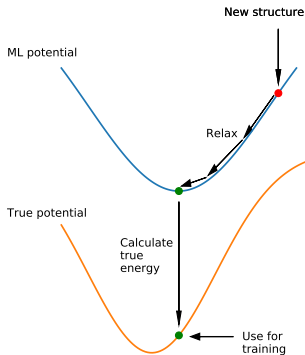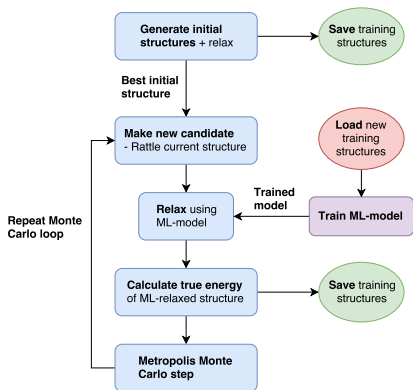

Diagram of the global search method

KRR/GPR

Prediction

$$E^*(\mathbf{x}^*) = \sum_i^N \alpha_i k(\mathbf{x}^*, \mathbf{x}_i) = \vec{\alpha}^T \vec{\kappa}$$

$$F^*(\mathbf{x}^*) = -\sum_i^N \alpha_i \frac{\partial k(\mathbf{x}^*, \mathbf{x}_i)}{\partial \mathbf{r}^*} = -\vec{\alpha}^T \nabla_{\mathbf{r}^*} \vec{\kappa}$$

Training

$$\vec{\alpha} = (\mathbf{K} + \lambda I)^{-1} \vec{E}$$

where $k(\cdot, \cdot)$ is the kernel function and $\mathbf{K}_{ij} = k(\vec{x_i}, \vec{x_j})$

Gaussian kernel

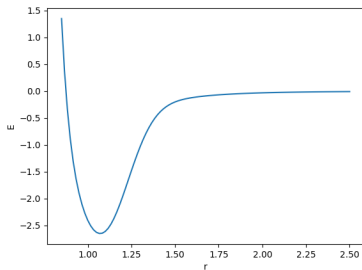$$k(\cdot, \cdot) = \exp\left(-\frac{d(\cdot, \cdot)^2}{2\sigma^2}\right)$$
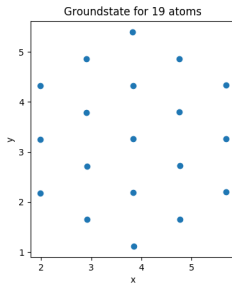
with the 2-norm for the dissimilarity d.

Feature

$$F_{A,B}(R) = \sum_{A_i, B_j} \frac{\delta(R - R_{ij})}{4\pi R_{ij}^2 \Delta\left(\frac{N_A N_B}{V}\right)}$$

$+$ an angular equivalent
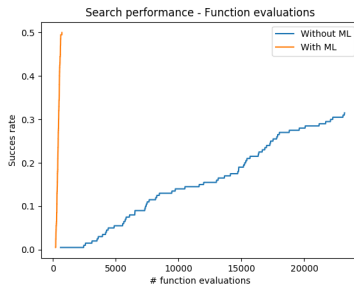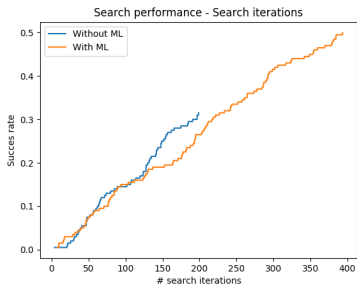
Model system - "Double" Lennard Jones

Interaction potential

Ground state for 19 atoms

Search results

Structures with 19 atoms

Structure check - prediction error

Filtering unresonable ML-relaxed structures

Rejection criteria:

$$\text{err}_{KRR} > ..$$

$$\frac{\text{err}_{KRR}}{\sqrt{\theta_0}} > ..$$