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Set 11 - Uncertainty Quantification for the N-body problem

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Question 1: Coupling with Pi4U

The Lennard-Jones potential has two parameters σ and ε, which we would like to infer from data. We propose to use available data of equation of state of liquid argon [1] in order to infer the above parameters.

The equation of state relates the state variables of the system: pressure, temperature and density. Here, we will measure the pressure given, as input, the temperature T and the density ρ, The temperature is set via the temperature rescaling thermostat you implemented in the previous exercise. The density is controlled by changing the size of the domain L and the number of particles N. The pressure can be computed from your simulations.

We model the data as

$$P_k = f(\varepsilon, \sigma \mid \rho_k, T_k) + e_k, \tag{1}$$

where $e_k \sim \mathcal{N}(0, s^2)$, and f is the computational model (your N-Body solver with Lennard-Jones potential, temperature rescaling and periodic boundary conditions).

In this exercise, we will infer ε and s for a fixed $\sigma = 0.34$ nm. Note that for convenience, we express ε in Kelvin units. This is done by expressing ε/k_B instead of ε.

a) Write down the likelihood, assuming your data is $D = \{T_k, \rho_k, P_k\}_{k=1}^n$.

Before running any simulation, we must make the data and the simulation units match. Here, we choose the following approach:

- fix length, time, temperature and mass scale
- define from these quantities an energy and a pressure scale
- convert all data quantities to simulation units

The unit scalings are described in Table.1. Note that the mass scaling is such that one Argon atom has mass 1 in the simulation.

It is then straightforward to convert physical units to simulation units. For example, if we choose to fix $\sigma = 0.34$ nm, we obtain, in simulation units, $\sigma^* = \sigma/l = 0.34$.

The available data is the temperature in `K`, the volume per mole in $\texttt{cm}^3/\texttt{mole}$, and the Pressure in `atm`.

Quantity	Simulation units	Physical units
length	$l^* = 1$	$l = 1$ nm
mass	$m^* = 1$	$m = 6.686376396 \times 10^{-26}$ kg
time	$t^* = 1$	$t = 5$ps
energy	$e^* = 1$	$e = m * l^2/t^2$
temperature	$T^* = 1$	$T = e/k_B$
pressure	$e^* = 1$	$e = e/l^3$
particle number	$N^* = N$	$N = 800$

Table 1: Units scalings between simulation and physical units. Simulation variables are denoted with a $.^*$

b) Compute the simulation temperature T^*_{eq} of the system. Complete the corresponding `TODO` in `skeleton/model/my_model.py`.

c) Compute the simulation length L^* of the box. This can be computed from the given volume per mole. Complete the corresponding `TODO` in `skeleton/model/my_model.py`.

d) Implement the log-likelihood evaluation in `skeleton/model/log_like.py`.

e) Run `tmcmc_theta_external` to sample from the posterior distribution. The prior information is described in `priors.par`, and configuration of TMCMC is described in `tmcmc.par`. The results can be visualized with the tool `pi4u/source/tools/display/plotmatrix_hist.py`.
You can use the tools as: `python plotmatrix_hist.py final.txt`, where `final.txt` contains the samplings generated by TMCMC.

References

[1] WB Streett and LAK Staveley. "Experimental study of the equation of state of liquid argon". In: *The Journal of Chemical Physics* 50.6 (1969), pp. 2302–2307.