Lab 5: Monte Carlo

SI1136 Simulation and Modeling

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5.1

5.1 Project

Use the Metropolis method to calculate

$$\langle x \rangle = \frac{\int_0^\infty x e^{-x} \, dx}{\int_0^\infty e^{-x} \, dx} . \tag{1}$$

Try different, also sufficiently large values of the parameter delta. Study σ/N and compare with the actual difference to the exact answer.[1]

[1] Note: N_0 is not critical when $x_0 = 0$.

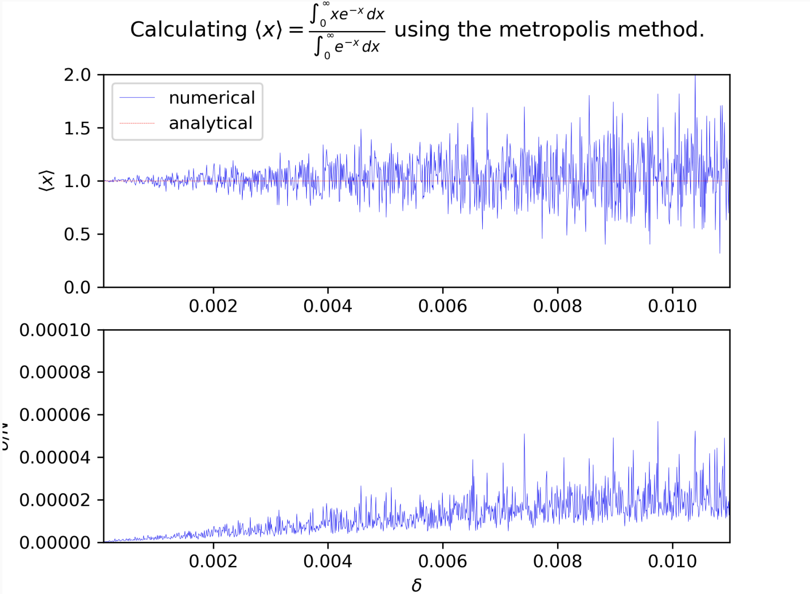
Exact value of the integral (1).

$$\langle x \rangle = \frac{\int_0^\infty x e^{-x}\,dx}{\int_0^\infty e^{-x}\,dx} = \frac{\overbrace{\left[-xe^{-x}\right]_0^\infty}^{0} + \int_0^\infty e^{-x}\,dx}{\int_0^\infty e^{-x}\,dx} = 1\ .$$

5.1 Method i

10 000 points are generated for $\delta = 0.0001, 0.0002, \ldots, 0.1$ after the first 100 points are thrown. Starting parameter $x_0 = 1$ since this is x_i should converge to.

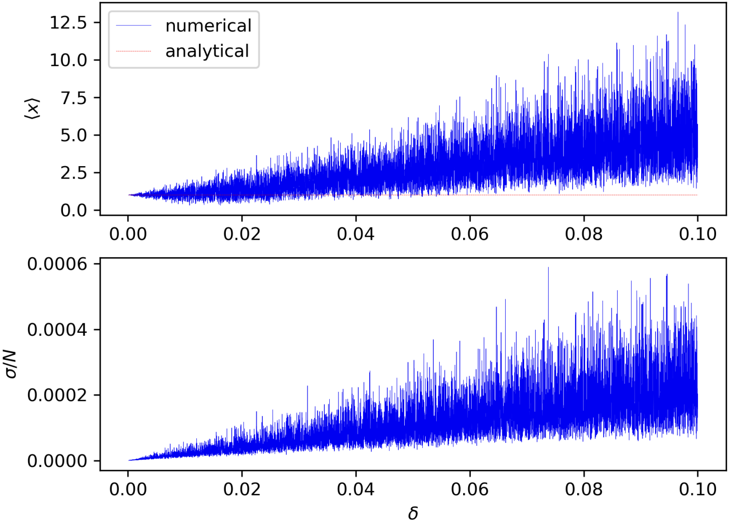
5.1 Results i



Calculating $\langle x \rangle = \frac{\int_0^\infty x e^{-x}\,dx}{\int_0^\infty e^{-x}\,dx}$ using the metropolis method.
numerical
analytical
$\langle x \rangle$
2.0
1.5
1.0
0.5
0.0
0.002
0.004
0.006
0.008
0.010
0.00010
0.00008
0.00006
0.00004
0.00002
0.00000
δ

5.1 Results ii

Calculating $\langle x \rangle = \frac{\int_0^\infty x e^{-x}\, dx}{\int_0^\infty e^{-x}\, dx}$ using the metropolis method.



5.1 Results iii

small $\boldsymbol{\delta}$: For small $\delta < 0.01, \langle x \rangle$ varies around the true value $\langle x \rangle = 1$.

large $\boldsymbol{\delta}$: For large $\delta > 0.01, \langle x \rangle$ increases linearly and fluctuates.

$\boldsymbol{\sigma / N}$: σ / N increases as δ increases (which is expected). σ / N is several (≈ 5) orders of magnitudes smaller than the actual difference to the exact answer. Since $N = 10\,000$, $\sigma \sim$ the actual difference to the exact answer.

5.2

5.2 Project

Implement the Lennard-Jones potential with $\sigma = 1$ and $\varepsilon = 1$ in the template. Try to find a large MC step size that gives reasonable acceptance. How does the step size affect the convergence of the energy?

Lennard-Jones potential.

The Lennard-Jones potential approximates the interaction between a pair of neutral atoms or molecules to the potential

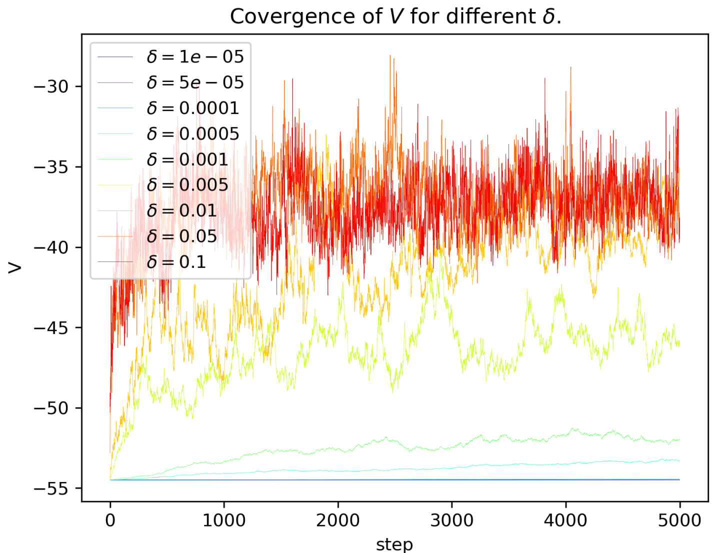
$$V_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] .$$

5.2 Method

A 5 000 step Monte-Carlo simulation is executed for each δ in

```
deltaArray = [0.00001, 0.00005, 0.0001, 0.0005,
        0.001, 0.005, 0.01, 0.05, 0.1] .
```

5.2 Results i



Covergence of V for different δ.
$\delta = 1e-05$
$\delta = 5e-05$
$\delta = 0.0001$
$\delta = 0.0005$
$\delta = 0.001$
$\delta = 0.005$
$\delta = 0.01$
$\delta = 0.05$
$\delta = 0.1$
V
step
−30
−35
−40
−45
−50
−55
0
1000
2000
3000
4000
5000

5.2 Results ii

small δ: Poor convergence. Small variance.

large δ: Good convergence. Large variance.

best δ: $0.05 < \delta < 0.1$.

5.3

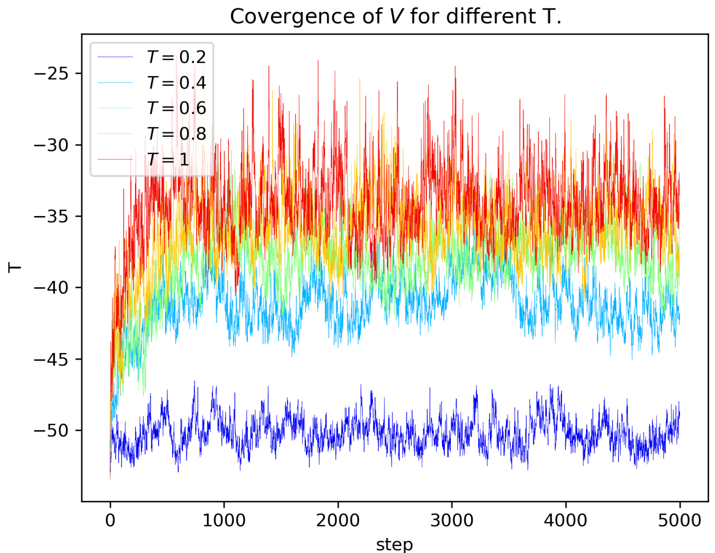
5.3 Project

Run LJ simulations at $T = 1$ and 0.2. What differences in collective behavior do you observe between 1 and 0.2 at long times? A physics question: can you explain what you see?

5.3 Method

A 5 000 step Monte-Carlo simulation is executed with $\delta = 0.05$ for each T in

`Tarray = [0.2, 0.4, 0.6, 0.8, 1]`.


Covergence of V for different T.
$T = 0.2$
$T = 0.4$
$T = 0.6$
$T = 0.8$
$T = 1$
−25
−30
−35
−40
−45
−50
T
0
1000
2000
3000
4000
5000
step

5.3 Results ii

convergence: Convergence is similar for all T.

small T: Small variance. Converges to small V.

large T: Large variance. Converges to large V.

physical interpretation: T is determined by the average kinetic energy of the particles. Large $T \implies$ higher movement $\implies$ more chaotic system. Furthermore, large T $\implies$ greater energy $\implies$ greater V.

5.4

5.4 Project

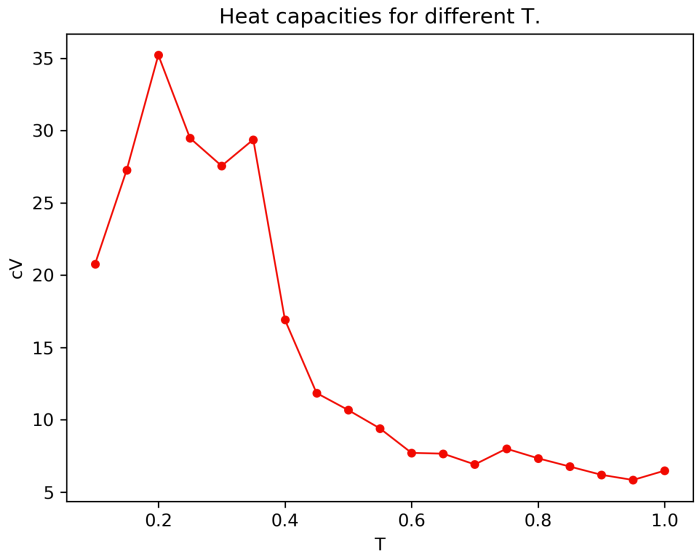
Use MC to calculate the average energy and heat capacity at several temperatures between $T = 0.2$ and 1. Can you explain the behavior of the heat capacity by looking at the sampled configurations?

The heat capacity is determined for T in

```
TArray = [0.1, 0.15, 0.2, ..., 1]
```

by averaging over $2\,000 \leq \text{step} \leq 10\,000$.

5.4 Results i



Heat capacities for different T.
cV
T
35
30
25
20
15
10
5
0.2
0.4
0.6
0.8
1.0

5.4 Results ii

The heat capacity decreases as the temperature increases.

Appendix

Source code

Available at:

https://github.com/axelstr/SI1336-Simulations-and-Modeling/tree/master/5%20Monte%20Carlo