Inference of inter-particle forces from stochastic trajectories

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System dynamics

- Langevin equation

$$dx = \frac{1}{\gamma} F(x)\, dt + \sigma \xi(t) dt$$

- $p(x_0, t_0), p(x_i, t_i \mid x_{i-1}, t_{i-1})$ – ?
- Fluctuation-dissipation theorem $D\beta\gamma = 1$
-

$$dx = D\beta F(x)\, dt + \sigma \xi(t) dt \tag{1}$$

Numerically generated trajectories

- Euler-Maruyama scheme
- Potentials

$$V_{HO}(x) = \frac{kx^2}{2} \tag{2}$$

$$V_{LJ}(x) = \epsilon \left[\left(\frac{r_{min}}{x} \right)^{12} - 2 \left(\frac{r_{min}}{x} \right)^{6} \right] \tag{3}$$

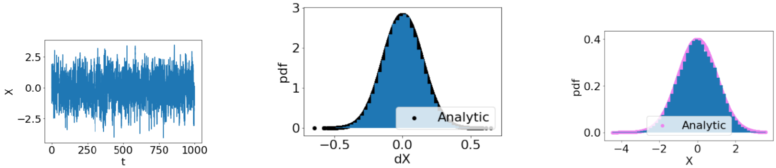
$$V_{dw-HO}(x) = k_4 \frac{x^4}{4} + k_3 \frac{x^3}{3} + k_2 \frac{x^2}{2} + k_1 x + k_0 \tag{4}$$

- Fitted displacement and position distributions

$$p\left(x\right) \propto \exp\left[-\beta V(x)\right] \tag{5}$$

$$p\left(x, t \mid x_0, t_0\right) \propto \exp\left[-\beta V(x - x_0)\right] \tag{6}$$

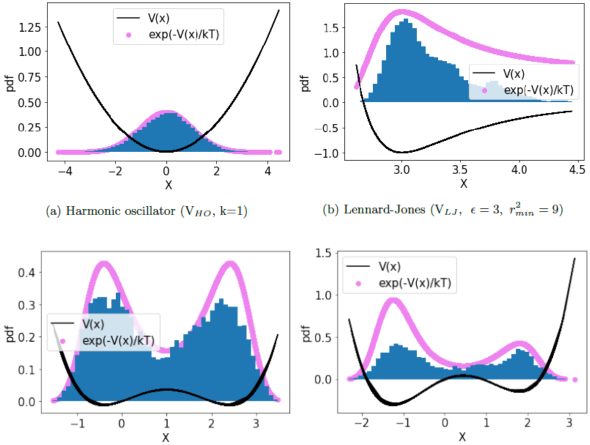
Harmonic Oscillator



(a) Trajectory (b) Distribution of displacement (c) Distribution of position

Figure 1.1: Stochastic trajectory of a particle in a harmonic oscillator potential

Position distribution



(a) Harmonic oscillator (V_{HO}, k=1)

(b) Lennard-Jones (V_{LJ}, $\epsilon = 3$, $r^2_{min} = 9$)

(c) Symmetric double-well HO (V_{dw-HO}, $k_1 = 1$, $k_2 = 1, k_3 = -3$, $k_4 = 1$)

(d) Asymmetric double-well HO (V_{dw-HO}, $k_1 = 1$, $k_2 = -2, k_3 = -1$, $k_4 = 1$)

Figure 1.2: Distribution of positions from stochastic trajectories

Theoretical aspects I

- Re-written eq 6, $d\omega(t) = \xi(t)dt$

$$dx = D\beta F\left(x\right)dt + \sigma d\omega(t)$$

- Average of eq. with the help of Itô lemma [2]

$$\begin{aligned} df[x(t)] =& f'[x(t)]a[x(t), t]dt + f'[x(t)]b[x(t), t]d\omega(t) \\ &+ \frac{1}{2}f''[x(t)](b[x(t), t])^2 dt \end{aligned}$$

- Fokker-Planck equation [2]

$$\partial_t p\left(x, t \mid x_0, t_0\right) = \left(\partial_x a \ + \frac{1}{2}\partial_x^2 \ b \ \right) p\left(x, t \mid x_0, t_0\right) \qquad (7)$$

Theoretical aspects II

- Postulates at thd. equilibrium for conservative force fields
  1. Boltzmann probability distribution
  2. No net flux of particles (probability)
- Fluctuation dissipation theorem [2]

$$\nabla D = \boldsymbol{F}(\boldsymbol{r})\left(\gamma^{-1} - D\beta\right) \tag{8}$$

- Smoluchowski equation

$$\partial_t p\left(x, t \mid x_0, t_0\right) = D\left(\partial_x^2 - \beta F(x)\right) p\left(x, t \mid x_0, t_0\right) \tag{9}$$

- Linear Potential $V(x) = cx$ [2]

$$p\left(x, t \mid x_0, t_0\right) = \frac{1}{\sqrt{4\pi D\left(t - t_0\right)}} \exp\left[-\frac{\left(x - x_0 + D\beta c\left(t - t_0\right)\right)^2}{4D\left(t - t_0\right)}\right] \tag{10}$$

Bayesian Inference

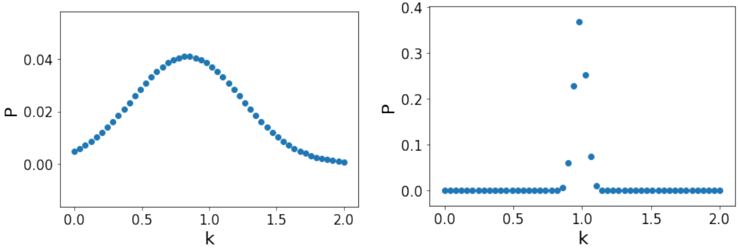
[1]

$$p\left(\theta \mid X\right)=\frac{p\left(X \mid \theta\right)\pi(\theta)}{p\left(X\right)}=\frac{\mathcal{L}_n(\theta)\pi(\theta)}{c_n} \tag{11}$$

$$c_n=p\left(X_1,\ldots,X_n\right)=\int \mathcal{L}_n(\theta)\pi(\theta)d\theta$$

- Parameters: $\theta=\{k_i\},\ i=1\ldots n$ from $F(\{k_i\})$, $X=dx_{i+1,i}$
- The likelihood: $\mathcal{L}_n(\theta)=\mathcal{N}\left(dx_{i+1,i}-F_i,\ 2D\Delta t\right)$
- The prior: $\pi(\theta)=\frac{1}{n}$

Results I

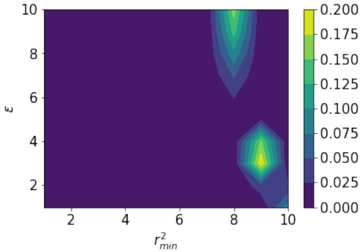


(a) $P(k)$ at step 9000

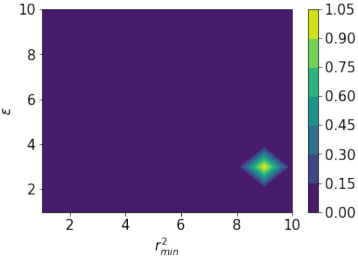
(b) $P(k)$ at the last step

Figure 1: Evolution of $P(k)$ for the HO case (Correct value $k = 1$)

Results II



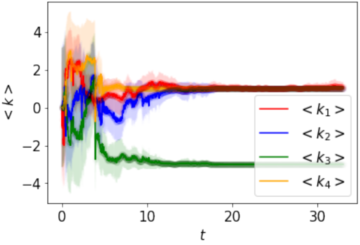
(a) $P(\epsilon; r^2_{min})$ at step 40



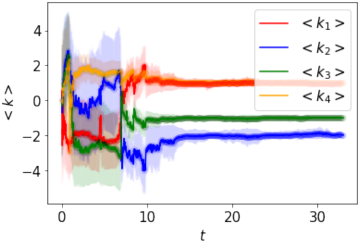
(b) $P(\epsilon; r^2_{min})$ at the last step

Figure 2: Evolution of $P(\epsilon; r^2_{min})$ for the LJ case (Correct values $\epsilon = 3; r^2_{min} = 9$)

Results III



(a)
$k_1 = 1, \; k_2 = 1, \; k_3 = -3, \; k_4 = 1$



(b)
$k_1 = 1, \; k_2 = -2, \; k_3 = -1, \; k_4 = 1$

Figure 3: Evolution of the inferred parameters and the diminishing standard deviation in time from the trajectories in the double-well HO

Conclusions

Advantages

- It works!
- No complicated Smoluchowski solution for $p(dX|F)$ needed
- Not all the data necessary

Disadvantages

- Slow with more parameters
- Analytic form of the forces needed
- A good guess of parameter intervals

References

H. Liu and L. Wasserman.
"Statistical Machine Learning", Chapter 12 .
2014.

K. Schulten.
"Lecture Notes PHYS498", Chapters 2,4,5.