On the statistics of a set of quantum mechanical harmonic oscillators. A machine learning approach.

Carlos Pegueros Denis

pegquerosdc@gmail.com

https://github.com/peguerosdc/ml4phy-quantum-oscillators

Brief introduction… from 0 to statistical physics

The energy eigenvalues of the quantum mechanical oscillator are given by:

$$\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

Which can be combined with the classical canonical distribution as a replacement for the Hamiltonian:

$$\rho_n = \frac{\exp\{-\beta\epsilon_n\}}{Z(T,V,1)}$$

$$\bar{E} = N\overline{\epsilon_n}$$

$$\overline{\epsilon_n} = \hbar\omega\left(\bar{n} + \frac{1}{2}\right)$$

$$\bar{n} = \frac{1}{\exp\{\beta\hbar\omega\} - 1}$$

Defining the neural network: Gaussian-Bernoulli RBM

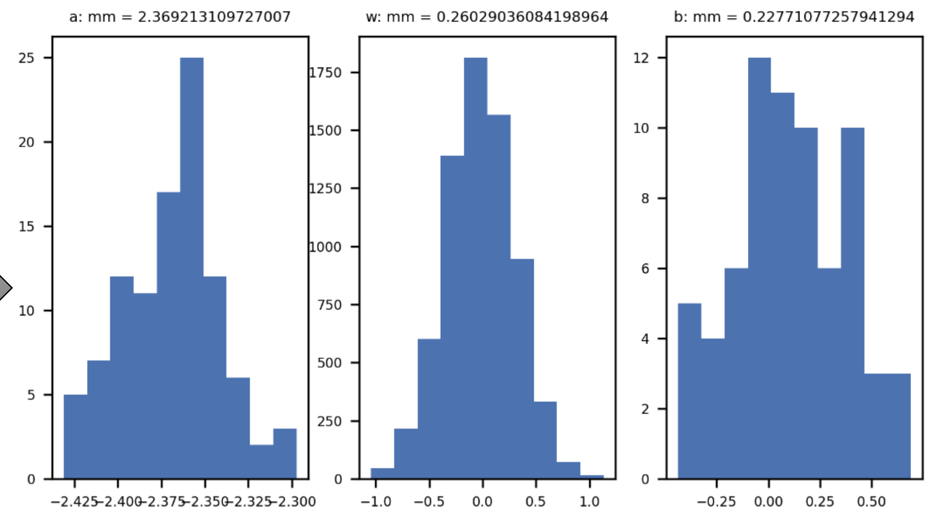
```
array([[0., 5., 0., 0., 3., 1., 0., 0.],
       [1., 0., 2., 1., 0., 0., 0., 0.],
       [1., 0., 1., 0., 0., 0., 0., 1.],
       [2., 1., 5., 0., 0., 0., 0., 0.],
       [2., 0., 0., 1., 0., 1., 0., 0.],
       [0., 1., 0., 0., 0., 0., 1., 0.],
       [0., 0., 2., 0., 0., 0., 1., 1.],
       [0., 1., 0., 0., 0., 2., 0., 2.]])
```

100k samples of 100 oscillators via Monte Carlo + ρ_n with:

- $T = 10 \times 10^{-6}\ [K]$
- $\omega = 1 \times 10^{-6}\ [rad/s]$

RBM

- 70 hidden units
- Batchsize = 10
- Learning rate = 0.005
- 300k training steps

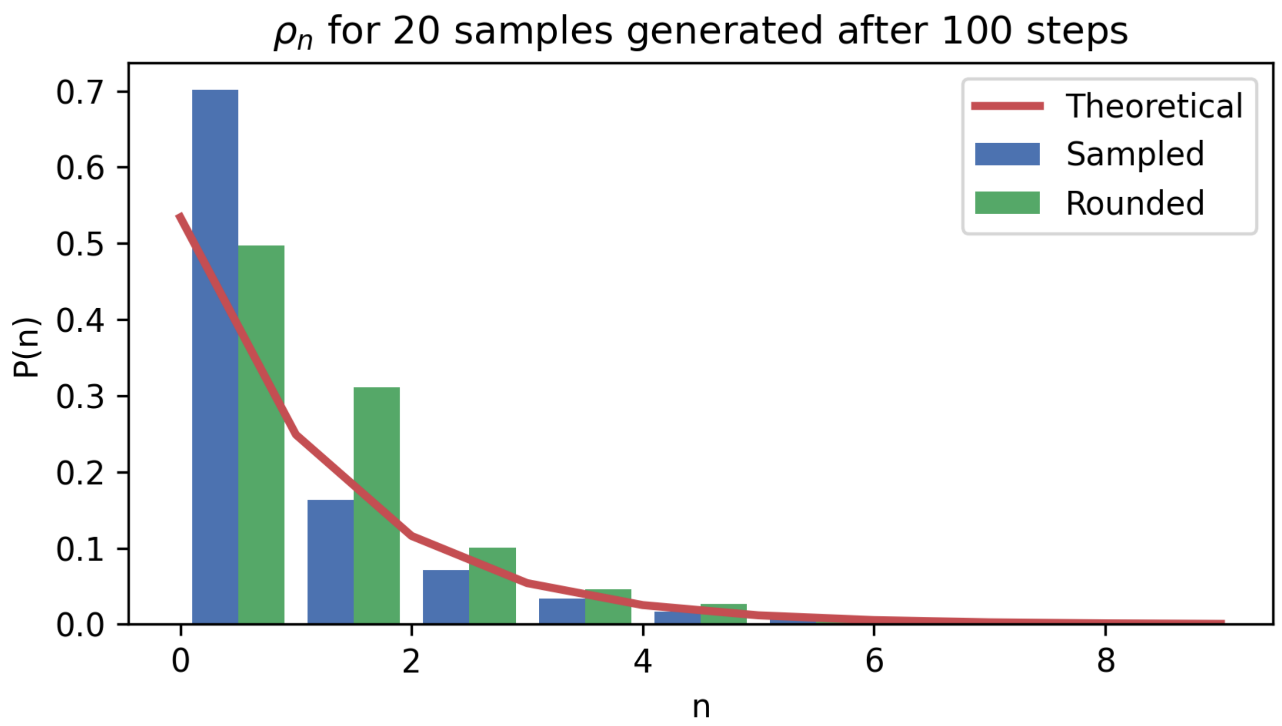


Does this predict $\bar{E},\ \overline{\epsilon_n},\ \bar{n}$?

Results

Two approaches considered:

1. Taking the **Sampled** quantum numbers generated by the Gaussian layer of the RBM. These can take any value from 0 to 1.
2. Denormalizing these sampled values and considering the **Rounded** values (to the closest integer) of these quantum numbers to get a "more physical result".



	Theoretical	Sampled	Rounded
$\bar{E}$ [J]	1.4471307636e-26	1.441212123e-26	1.3788526515e-26
$\overline{\epsilon_n}$ [J]	1.4471307636e-28	1.4412121231e-28	1.3788526515e-28
$\bar{n}$	0.872244867016	0.866632503412	0.8075