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Computational Physics – Exercise 5

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1 Artificial Hamiltonian and Equations of Motion

We have the integral,

$$\frac{1}{Z}\int_{-\infty}^{\infty} d\phi \cos\left(\sqrt{1+\phi^2}\right)\frac{e^{-\phi^2}}{2+\phi^2} \equiv \left\langle \cos\left(\sqrt{1+\phi^2}\right)\right\rangle \tag{1}$$

Now we bring the $2+\phi^2$ term into the exponential by,

$$\frac{1}{Z}\int_{-\infty}^{\infty} d\phi \cos\left(\sqrt{1+\phi^2}\right) e^{-\phi^2-\ln(2+\phi^2)} \equiv \left\langle \cos\left(\sqrt{1+\phi^2}\right)\right\rangle \tag{2}$$

Thus, our artificial Hamiltonian reads as,

$$\mathcal{H}(p,\phi) = \frac{p^2}{2} + \phi^2 + \ln(2+\phi^2) \tag{3}$$

Now we use Hamilton's equations to calculate the equations of motion,

$$\dot{\phi} = p \tag{4}$$

$$\dot{p} = -2\phi - \frac{2\phi}{2+\phi^2} \tag{5}$$

2 Normalized autocorrelation function

The normalized autocorrelation function is given by

$$\Gamma^O(t) = \frac{C^O(t)}{C^O(0)} \tag{6}$$

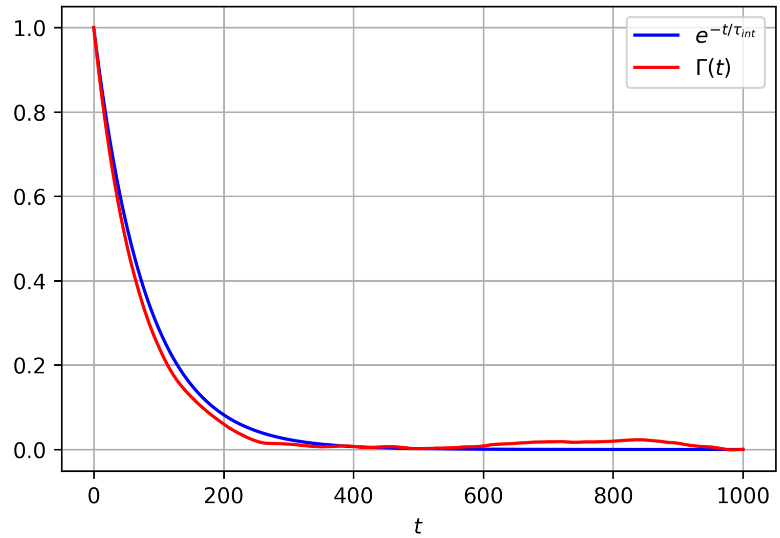
where,

$$C^O(t) = \frac{1}{N - |t|} \sum_{i=1}^{N-|t|} (O_i - \bar{\mu}) \left(O_{i+|t|} - \bar{\mu}\right) \tag{7}$$

With these in hand we define the normalized autocorrelation time to be

$$\tau_{int} \approx \frac{1}{2}\Gamma(0) + \sum_{t=1}^{W} \Gamma(t) \tag{8}$$

The code these can be found at [1]. We now compare the autocorrelation function that we obtain with $e^{-t/\tau_{\text{int}}}$ for $t \geq 0$ in figure 2.



3 Autocorrelation and Bin width

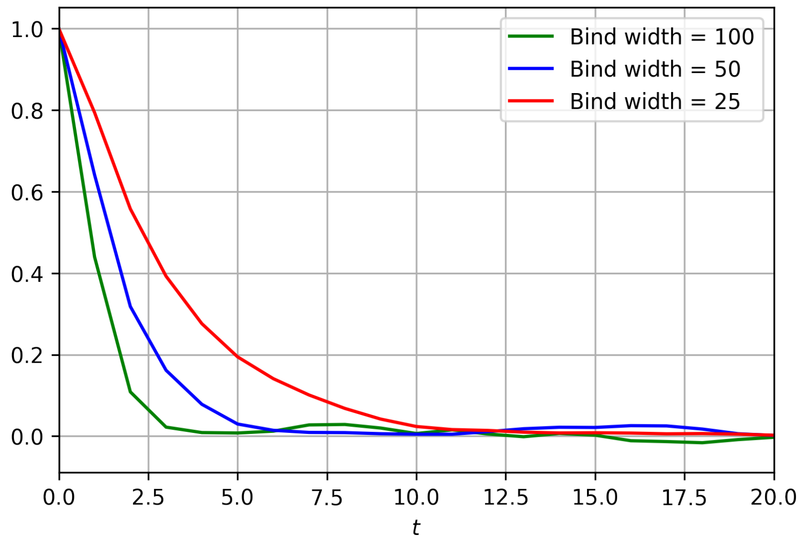
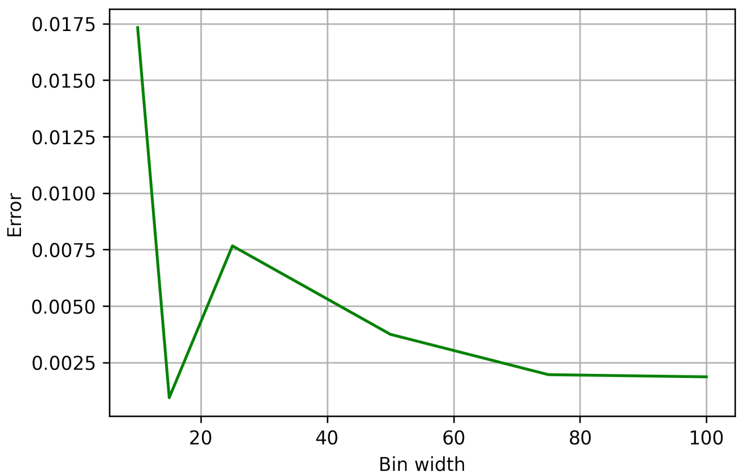


Figure 1: We can see that autocorrelation decreases as the bin width is increased.. Comparing this to figure 2, we can also see integrated autocorrelation time has has decreased by at least a factor of 10

4 Behavior of the error as a function of bin width



5 Error as a function of the ensemble size

We choose a bin width of 75.

Figure 2: Caption

References

[1] P. Anancia Devaneyan and R. K. Senthilkumar. Exercises for the Physics 760: Computational Phyics course during the WS 22/23 Term.