Institute for Cross-Disciplinary Physics and Complex

Task 3

Simulation Methods

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1 Exercise 78

In this exercise, we will generate $M = 10^6$ random numbers distributed according a Gaussian distribution of mean 0 and variance 1 using the Metropolis algorithm. We will use this series of values to evaluate the functions $G_1(x) = x^2$ and $G_2(x) = \cos(x)$ and compute the correlation function $\rho_G(k)$ which is shown in Fig 1. Using the correlation function, we will compute the correlation time τ_G using

$$\tau_G = \sum_{k=1}^{1000} \rho_G(k) \ , \quad \tau_G \approx \tau_{G,1} = \frac{\rho_G(1)}{1 - \rho_G(1)}. \tag{1}$$

Results for the correlation time are summarized in Tab. 1.The exponential approximation yields a slightly different value, yet both results share the same order of magnitude. Thus, the exponential approach can be considered as a good approximation for the correlation time.

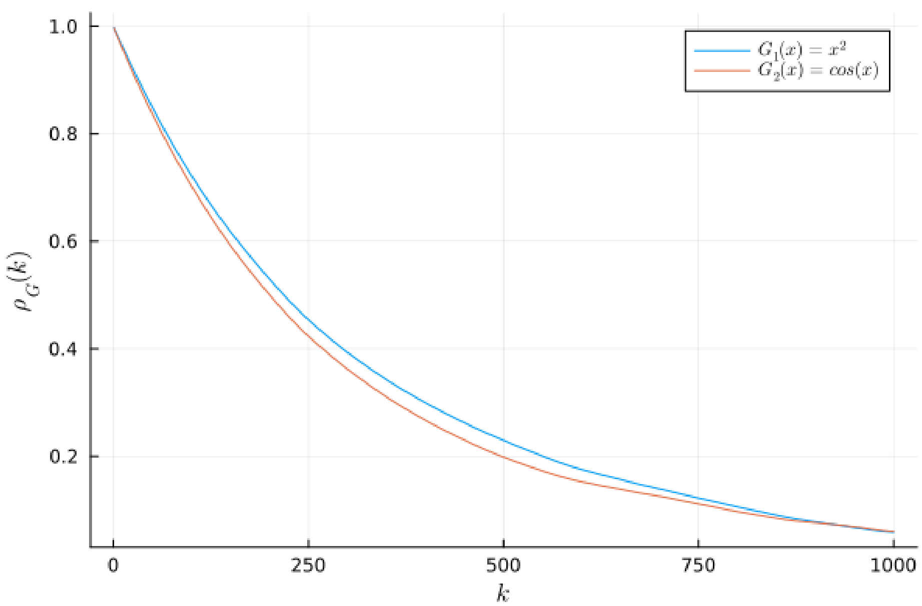

Figure 1: Correlation function $\rho_G(k)$ for $G_1(x) = x^2$ and $G_2(x) = \cos(x)$ and $k \in [0, 1000]$.

$G(x)$	τ_G	$\tau_{G,1}$
$G_1(x) = x^2$	317.211	310.166
$G_2(x) = \cos(x)$	297.913	279.504

Table 1: Results for the correlation time.

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We aim to compute the value of the integrals

$$I_1 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{2}} \ , \ \ I_2 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \cos(x) e^{-\frac{x^2}{2}}$$

using the random number generator of the previous exercise. The value of each integral is obtained by calculating the average of $G_1(x) = x^2$ and $G_2(x) = \cos(x)$ using $M = 10^6$ random numbers following a Gaussian distribution of mean 0 and variance 1. The error of this calculation is

$$\sigma^2[\hat{G}] = \frac{1}{M}\sum_{i=1}^{M} G(\hat{\mathbf{x}}_\mathbf{i})^2 - \left(\frac{1}{M}\sum_{i=1}^{M} G(\hat{\mathbf{x}}_\mathbf{i})\right)^2 \ , \ \ \sigma^2[\mu_M[G]] = \frac{\sigma^2[\hat{G}]}{M}(2\tau_G - 1).$$

Nevertheless, in other to see the effect of the correlation time on the error we will compute

$$\epsilon_C \equiv \sigma^2[\mu_M[G]] = \frac{\sigma^2[\hat{G}]}{M}(2\tau_G - 1) \ , \ \ \epsilon \equiv \sigma^2[\mu_M[G]] = \frac{\sigma^2[\hat{G}]}{M}$$

where ϵ is the error for uncorrelated variables. The results are summarized in Tab 2. We can see that ϵ and ϵ_C are significantly different.Thus, it is important to take into account the correlation time in order to not underestimate the errors. Using ϵ, the numerical outcomes do not align with the exact values within the expected margin of errors. This discrepancy, however, is rectified by accounting for errors stemming from the correlation of random numbers.

I_i	$\langle G_i \rangle$	ϵ_C	ϵ	$I_{i,th}$
I_1	0.981	0.035	0.0014	1.0
I_2	0.611	0.011	0.00044	0.60608

Table 2: Value of the integrals with their corresponding error and the exact value $I_{i,th}$.