KFU Graz
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CP1: Monte Carlo Methods WS 2023/24

8. Exercise: Generating random numbers with Maxwell-Boltzmann Distribution

The probability density of the Maxwell-Boltzmann distribution is given by

$$P(x) = \sqrt{\frac{2}{\pi}} \frac{x^2 e^{-x^2/(2a^2)}}{a^3}, \qquad x > 0 \tag{1}$$

Generate random numbers $x_i \in [0, 10]$ with this distribution (take $a = 1$) using the rejection method starting from a uniform distribution. What C is needed? What is the rejection rate? Calculate the mean,variance and skewness with errors and verify they agree with the exact results.

$$\mu = 2a\sqrt{\frac{2}{\pi}}, \qquad \sigma^2 = \frac{a^2(3\pi - 8)}{\pi}, \qquad \gamma_1 = \frac{2\sqrt{2}(16 - 5\pi)}{(3\pi - 8)^{3/2}} \tag{2}$$

The skewness if defined as

$$\gamma_1 = \frac{\langle (x-\mu)^3 \rangle}{\langle (x-\mu)^2 \rangle^{3/2}}, \qquad \text{with } \mu = \langle x \rangle. \tag{3}$$

To calculate errors for variance (skeweness) generate e.g. 50 samples with a sample size of 10^6, and calculate the variance (skewness) for all of them, giving you a 50 element sample of the variance (skewness). Now you can calculate the errors as usual (for example using your subroutine from Exercise 4).
Try again by starting from Gauss distributed random numbers with mean=2, sigma=1, $C = 2.1$. What is the new rejection rate?

9. Exercise: Generating random numbers with Maxwell-Boltzmann Distribution

Set up a Metropolis Markov chain to generate random numbers according to the Maxwell-Boltzmann distribution, given by (use $a = 1$)

$$P(x) = \sqrt{\frac{2}{\pi}} \frac{x^2 e^{-x^2/(2a^2)}}{a^3}, \qquad x > 0. \tag{4}$$

The proposal step can use $x \to x + \eta$, where η is a Gaussian random number with a given variance σ.
Try different σ values and see how the acceptance rate depends on that.
Calculate the mean and variance with errors and verify that they agree with the exact results.

$$\mu = 2a\sqrt{\frac{2}{\pi}}, \qquad \sigma^2 = \frac{a^2(3\pi - 8)}{\pi}, \qquad \gamma_1 = \frac{2\sqrt{2}(16 - 5\pi)}{(3\pi - 8)^{3/2}} \tag{5}$$

What happens if you use a non-symmetric proposal distribution?
Hint: Gaussian random numbers in numpy: (`numpy.random.normal(loc=mean,scale=sigma)`)
bonus question: Calculate the autocorrelation time of the resulting random variable.

8. Exercise: Independence Metropolis sampler

On the lecture we discussed that in the Metropolis alg. we need the following acceptance probability of a proposed step

$$T_A(\Phi'|\Phi) = \min\left(1, \frac{T_0(\Phi|\Phi')\pi(\Phi')}{T_0(\Phi'|\Phi)\pi(\Phi)}\right) \tag{6}$$

Where $T_0(\Phi'|\Phi)$ is the proposal probability and $\pi(\Phi)$ is the desired equilibrium distribution. Instead of choosing a symmetric proposal, now we do the following: suppose we have a random generator for the distribution $\pi_{approx}(\Phi)$. We than choose $T_0(\Phi'|\Phi) = \pi_{approx}(\Phi')$, i.e. we take samples from this generator as proposals independently of the current Φ. Now the acceptance probability should be:

$$T_A(\Phi'|\Phi) = min\left(1, \frac{\pi_{approx}(\Phi)\pi(\Phi')}{\pi_{approx}(\Phi')\pi(\Phi)}\right) \tag{7}$$

Set up a Metropolis Markov chain to generate random numbers according to the Maxwell-Boltzmann distribution, given by (use $a = 1$)

$$P(x) = \sqrt{\frac{2}{\pi}}\frac{x^2 e^{-x^2/(2a^2)}}{a^3}, \qquad x > 0. \tag{8}$$

We use the gaussian distribution $\pi_{approx}(x) \simeq e^{-x^2/(2a^2)}$ for the proposals, and we correct for the x^2 factor using the above mentioned process.
Calculate the mean and variance with errors and verify that they agree with the exact results.

$$\mu = 2a\sqrt{\frac{2}{\pi}}, \qquad \sigma^2 = \frac{a^2(3\pi - 8)}{\pi}, \qquad \gamma_1 = \frac{2\sqrt{2}(16 - 5\pi)}{(3\pi - 8)^{3/2}} \tag{9}$$

What is the acceptance rate? How could one improve on that?