CP Test 1 KDSMIL001 14-05-2022

1. (a) We begin, when integrating using Gauss-Laguerre quadrature, by transforming the integrals in question,

$$I = \frac{\int_0^\infty (x^4 + 1)xe^{-\sqrt{4x^2 + 1}}dx}{\int_0^\infty xe^{-\sqrt{4x^2 + 1}}dx}$$
(1)

into ones of the form

$$\int_0^\infty f(x)e^{-x}.\tag{2}$$

We begin with the numerator, which we will call I_N . Choosing the substitution $w = \sqrt{4x^2 + 1}$, we get

$$x = \sqrt{\frac{w^2 - 1}{4}}, \quad x^4 + 1 = \left(\frac{w^2 - 1}{4}\right)^2 + 1, \quad dx = \frac{w}{2\sqrt{w^2 - 1}}dw$$

Then we find

$$I_N = \int_1^\infty \frac{w}{2\sqrt{w^2 - 1}} \left(\left(\frac{w^2 - 1}{4} \right)^2 + 1 \right) \sqrt{\frac{w^2 - 1}{4}} e^{-w} dw$$
$$= \int_0^\infty \frac{w}{4} \left(\left(\frac{w^2 - 1}{4} \right)^2 + 1 \right) e^{-w} dw$$

Using another substitution, x = w - 1, we can see

$$I_N = \int_0^\infty \frac{x+1}{4} \left(\left(\frac{x^2 + 2x}{4} \right)^2 + 1 \right) e^{-x-1} \tag{3}$$

where we easily identify

$$f_N(x) = \frac{x+1}{4e} \left(\left(\frac{x^2 + 2x}{4} \right)^2 + 1 \right).$$
 (4)

For the denominator, we use the same two substitutions, finding

$$I_D = \int_0^\infty x e^{-\sqrt{4x^2 + 1}} dx$$

$$= \int_1^\infty \frac{w}{4} e^{-w} dw$$

$$= \int_0^\infty \frac{x + 1}{4e} e^{-x} dx$$
(5)

$$\implies f_D(x) = \frac{x+1}{4e}.\tag{6}$$

We can then use Gauss-Laguerre quadrature to find these integrals:

$$I_N \approx \sum_{i=1}^n f_N(x_i) w_i \tag{7}$$

$$I_D \approx \sum_{i=1}^n f_D(x_i) w_i \tag{8}$$

(b) For a Monte Carlo integration method, we choose the Metropolis method, as the integral in equation (1) is of the form

$$I = \frac{\int p(x)f(x)dx}{\int p(x)dx}.$$
 (9)

We can identify $f(x) = x^4 + 1$, and thus we need to sample according to

$$p(x) = xe^{-\sqrt{4x^2 + 1}}. (10)$$

Using the Metropolis method allows us to not have to normalise this p(x), which is nice as the integral of it is a bit ugly.

To begin with, we generate $N_0 = 500\,000$ points x_i , according to p(x) using the Metropolis random walk/Markov chain method. In order to avoid correlation between points we compute the autocorrelation function

$$C(j) = \frac{\langle x_{i+j}x_i \rangle - \langle x_i \rangle^2}{\langle x_i^2 \rangle - \langle x_i \rangle^2}$$
(11)

for a range of j values, and find the first j for which $C(j) \leq 0.01$.

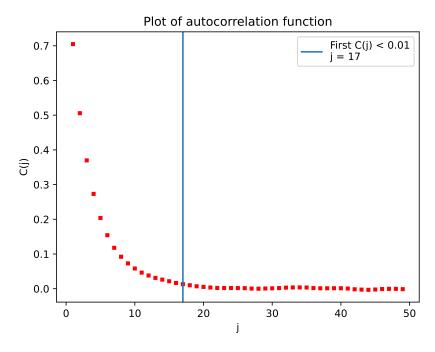


Figure 1: Plot of the autocorrelation function for the N_0 generated values, giving us C(j = 17) as the first value ≤ 0.01 .

This tells us how many numbers in the Markov chain to skip each time we choose one to be part of our final distribution. We also need to consider the starting values, as the method goes through a transient phase before equilibrating. To find how many numbers to chop off the start, we can find the moving average of the N_0 generated values, and see when it begins to level level off.

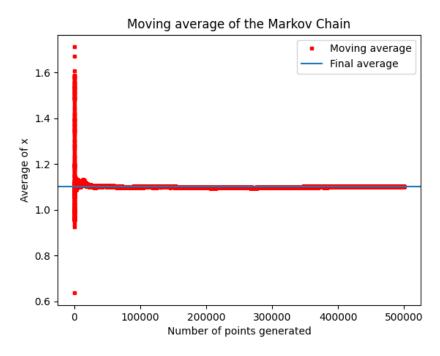


Figure 2: Plot of the moving average of the N_0 points in the generated Markov chain, along with the final average, to see when the moving average begins to level off.

By inspection, we can see it levels off at around $20\,000$ points, so we choose to cut off the first $20\,000$ points. Doing this and skipping every 17 points leaves us with around $28\,000$ points in our distribution.

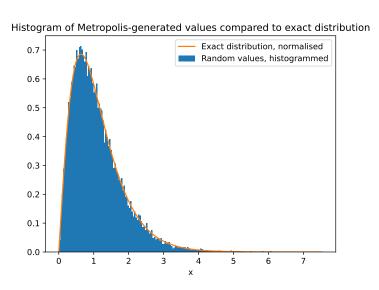


Figure 3: Histogram of the x-values calculated using the Metropolis method, distributed according to equation (10), along with the exact distribution. Note that the histogram is normalised to 1 over the interval shown, while p(x) is normalised over the semi-infinite interval, so there may be some discrepancies.