Computational Physics II
Spring 2021

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Integration using Metropolis Algorithm

Contents

1 Question Formulation and Analytical solution

The integral of the function,

$$f(x) = (x^2 + x) \cdot e^{-x}$$

is to be calculated over the interval $[1, 5$ using metropolis algorithm.

To check the correctness of the implementation, the analytical result can be first evaluated.

$$I = \int_1^5 f(x) dx$$

The solution to the above integral is:

$$I = \mathrm{e}^{-5} \left(7\mathrm{e}^4 - 43\right) = 2.28542436$$

2 Implementation and Results

The metropolis algorithm was implemented and the integral was evaluated using three different probability distribution functions

$$p_a(x) = 1$$
$$p_b(x) = e^{-x}$$
$$p_c(x) = (x^2 + x)e^{-x}$$

and three different values maximum step size, $\delta = [2, 2.5, 3]$

2.1 Histograms

The graph the function in the concerned domain is shown in figure (1).

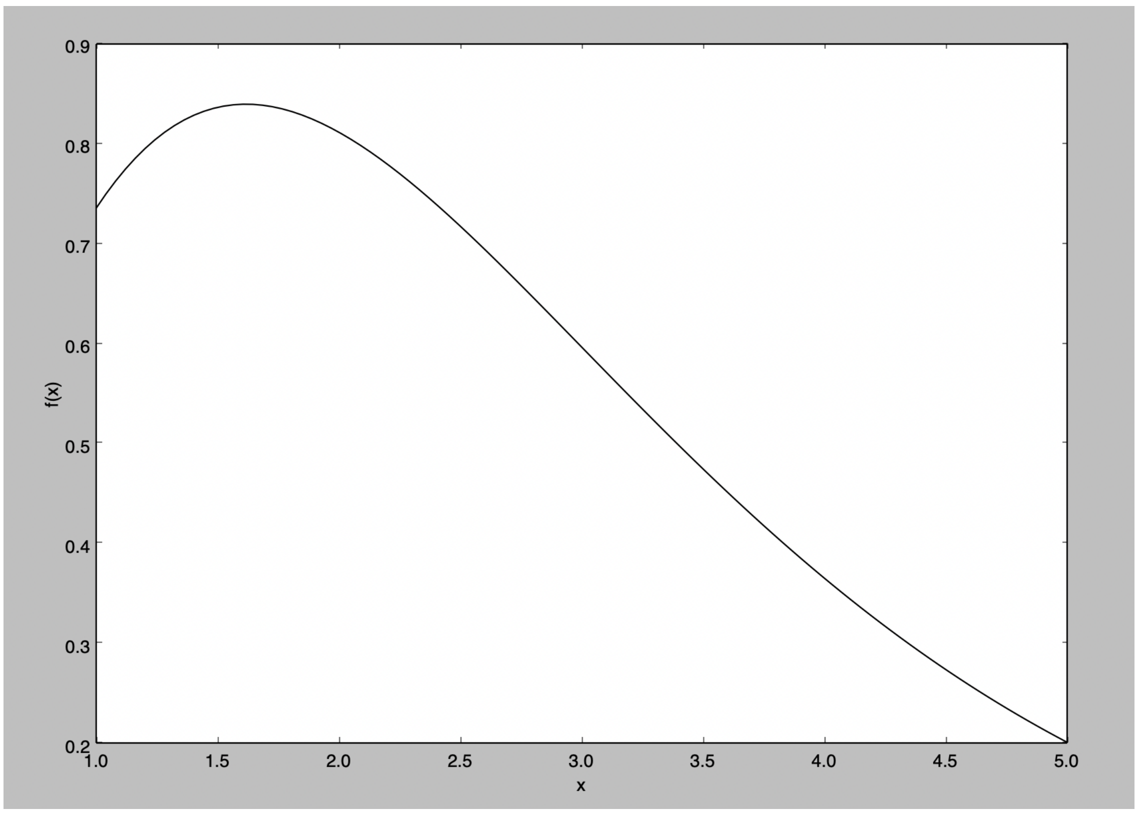

Figure 1: Graph of function

2.1.1 p_a with $\delta = 2$

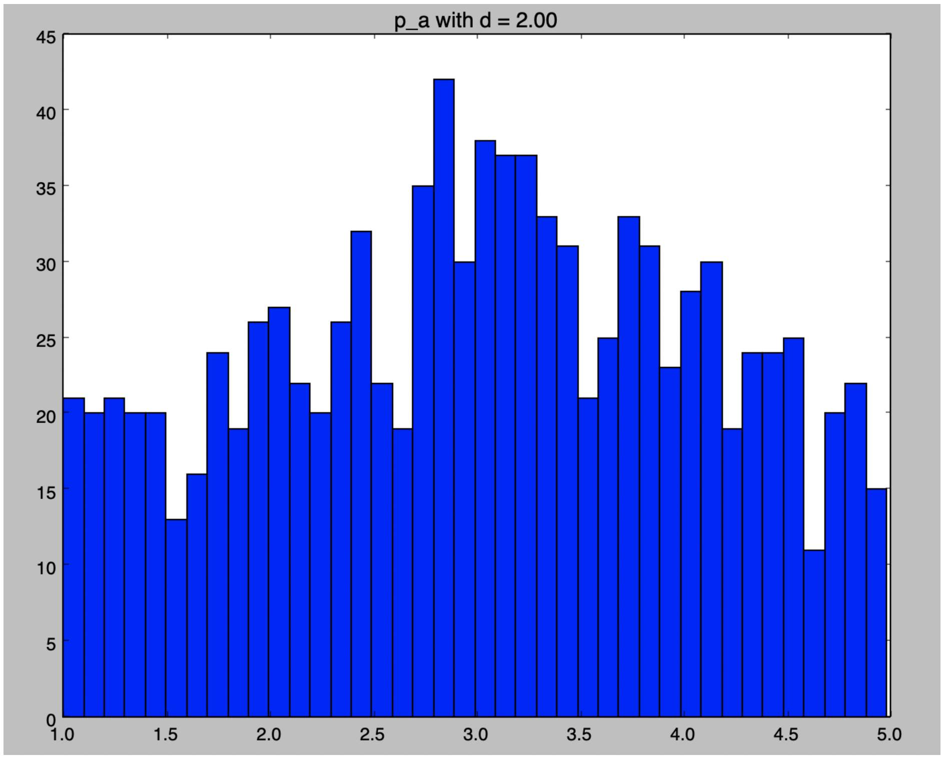

Figure 2: Histogram distribution using p_a with $\delta = 2$

2.1.2 p_a with $\delta = 2.5$

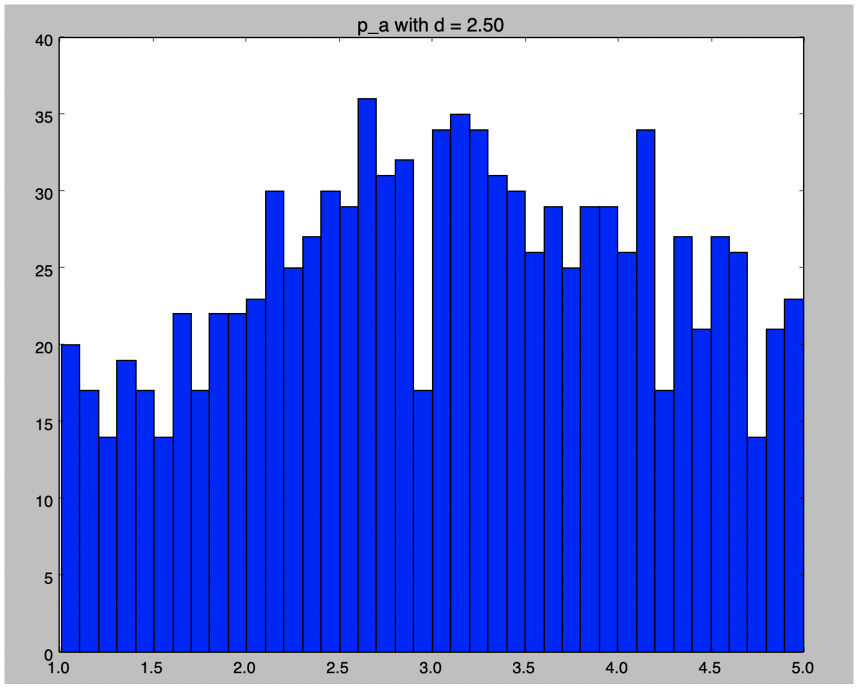

Figure 3: Histogram distribution using p_a with $\delta = 2.5$

2.1.3 p_a with $\delta = 3$

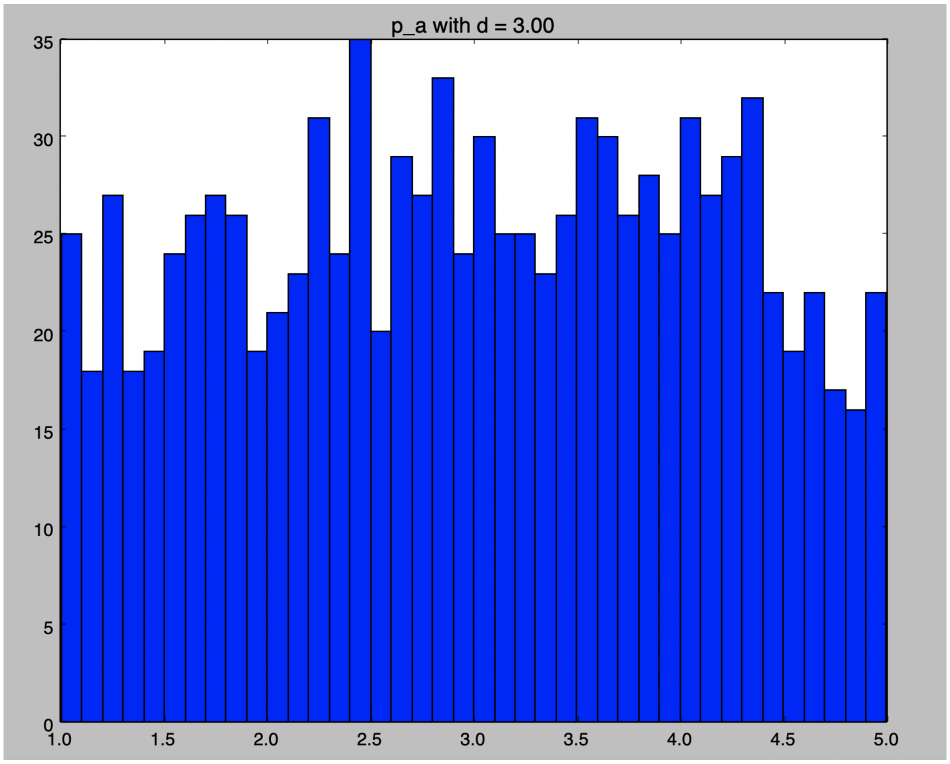

Figure 4: Histogram distribution using p_a with $\delta = 3$

2.1.4 p_b with $\delta = 2$

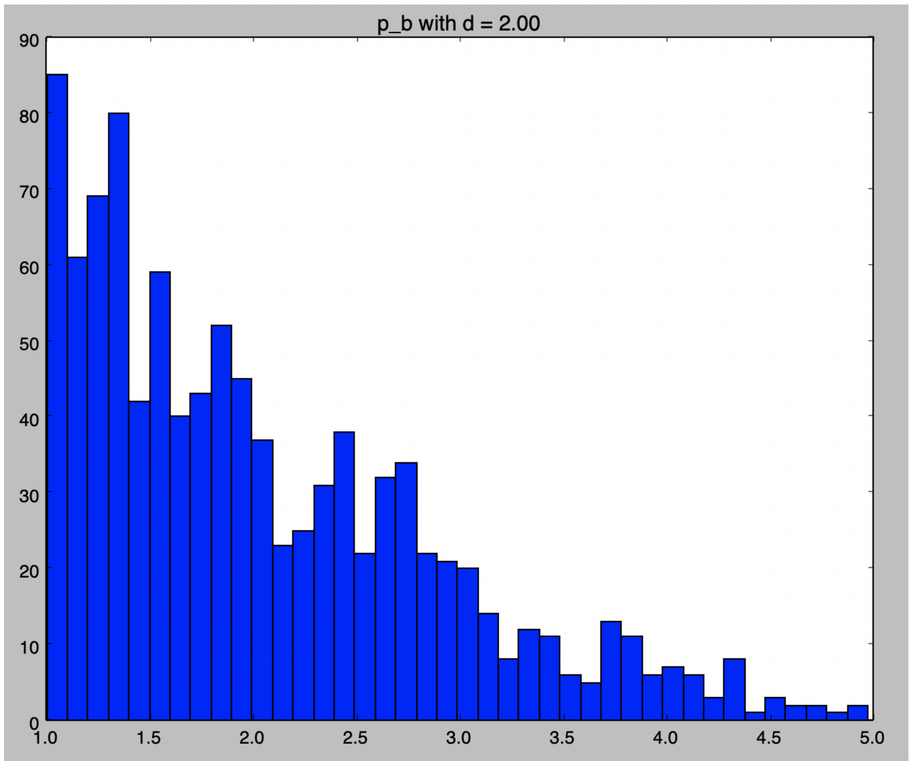

Figure 5: Histogram distribution using p_b with $\delta = 2$

2.1.5 p_b with $\delta = 2.5$

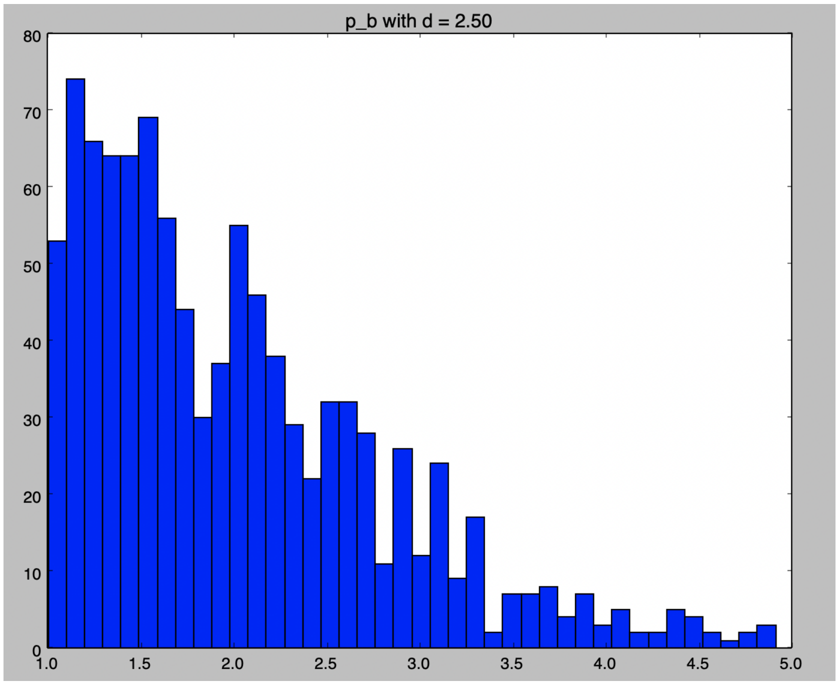

Figure 6: Histogram distribution using p_b with $\delta = 2.5$

2.1.6 p_b with $\delta = 3$

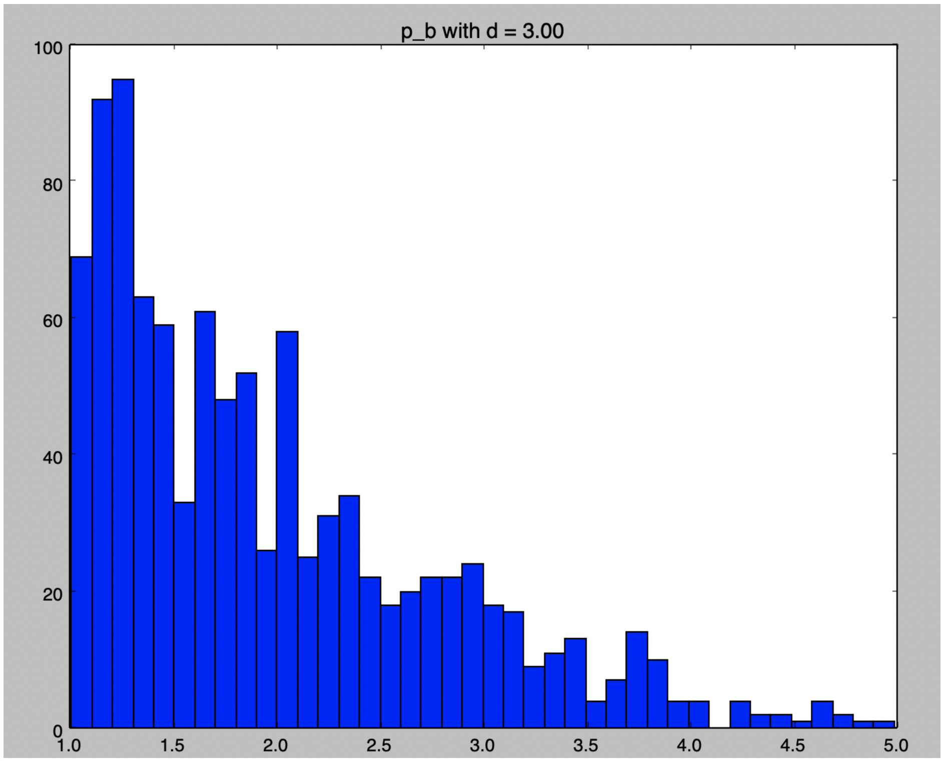

Figure 7: Histogram distribution using p_b with $\delta = 3$

2.1.7 p_c with $\delta = 2$

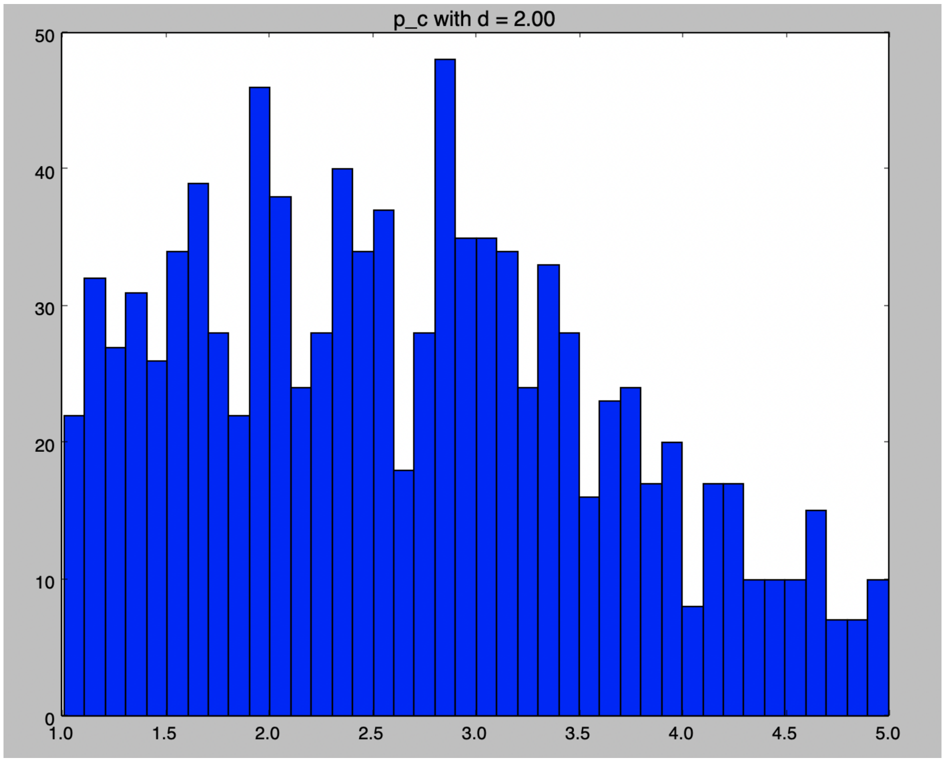

Figure 8: Histogram distribution using p_c with $\delta = 2$

2.1.8 p_c with $\delta = 2.5$

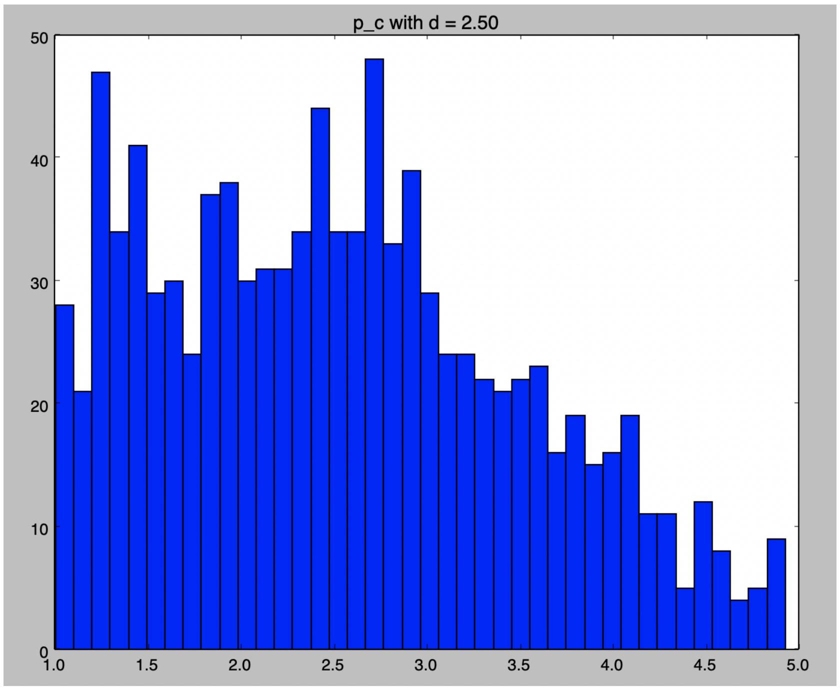

Figure 9: Histogram distribution using p_c with $\delta = 2.5$

2.1.9 p_c with $\delta = 3$

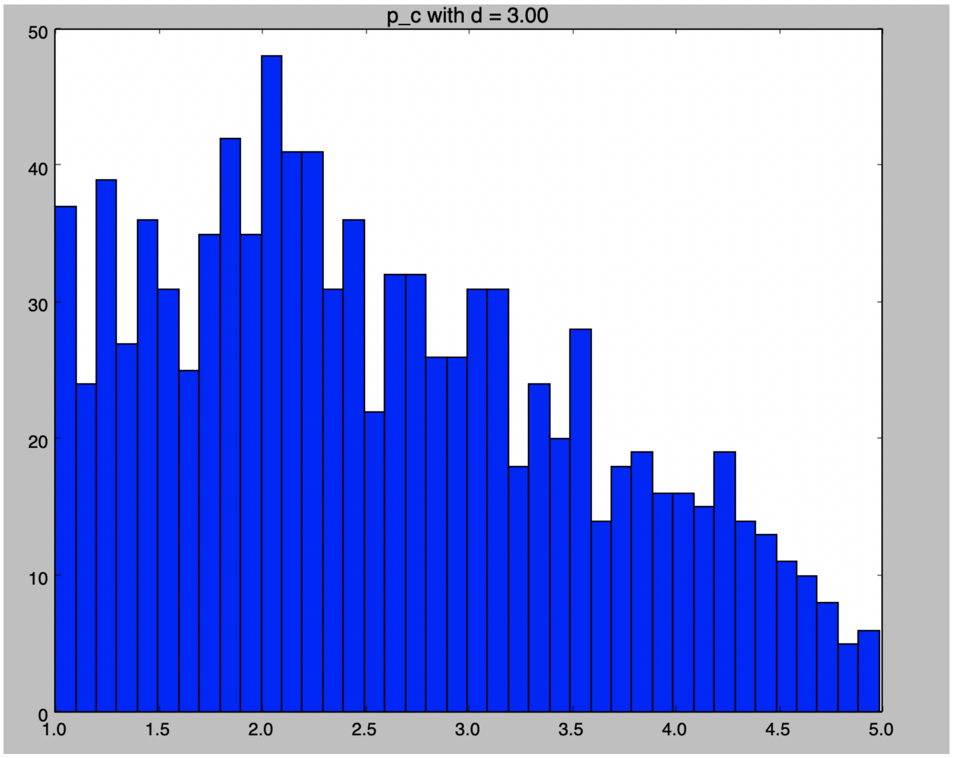

Figure 10: Histogram distribution using p_c with $\delta = 3$

2.2 Comparison with analytical solution

2.2.1 At $\delta = 2$

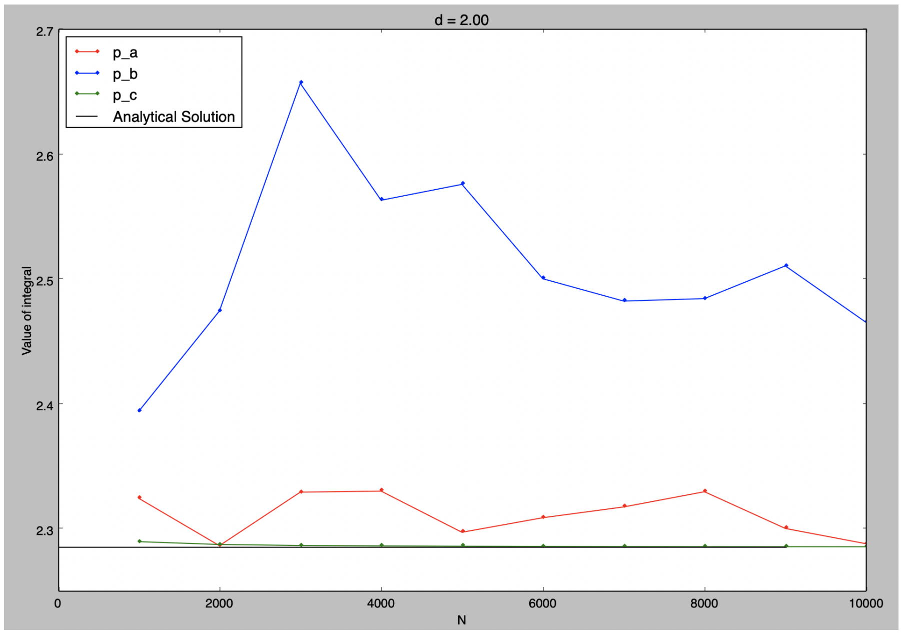

Figure 11: Evaluated integral with different probability distributions at $d = 2$

2.2.2 At $\delta = 2.5$

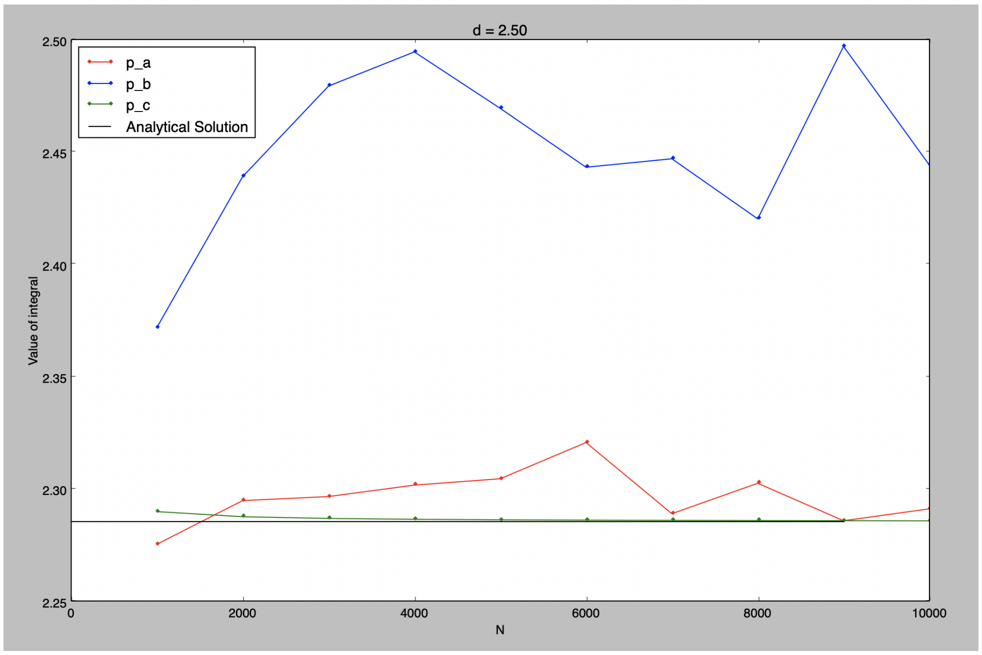

Figure 12: Evaluated integral with different probability distributions at $d = 2.5$

2.2.3 At $\delta = 3$

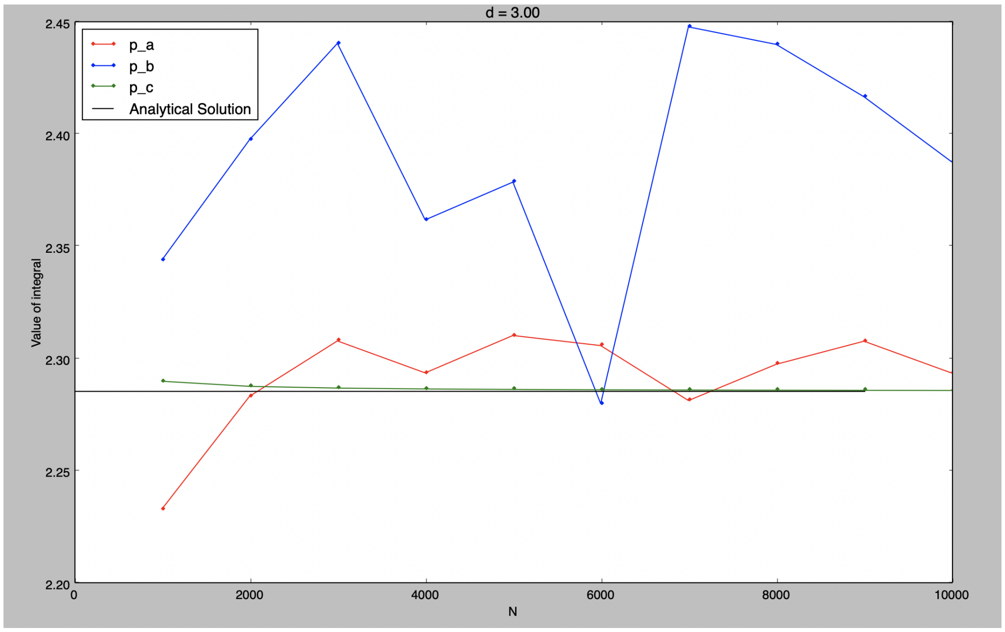

Figure 13: Evaluated integral with different probability distributions at $d = 3$

The above plots are be summarised in plot (14).

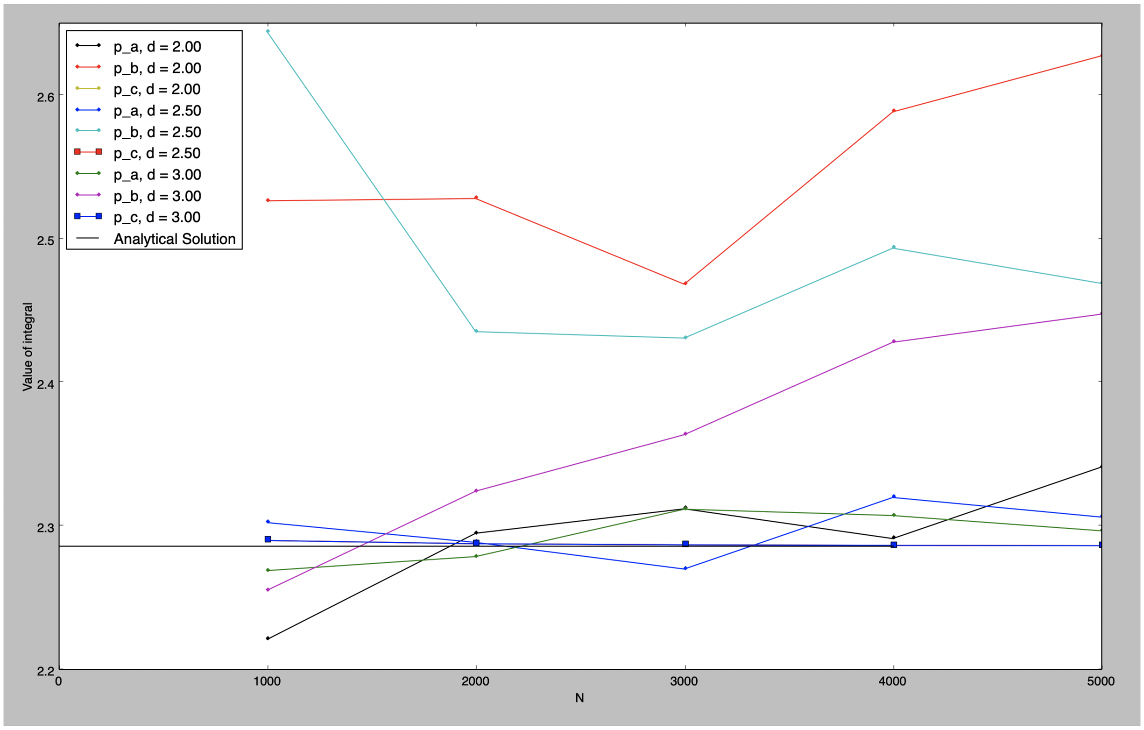

Figure 14: Evaluated integral with different probability distributions

3 Conclusion

As seen from the above plots, it can be concluded the integral evaluated using metropolis algorithm converged for the probabilities distribution defined by $p_c(x)$ as well as $p_a(x)$. However, the results obtained using the distribution defined by $p_b(x)$ deviates considerably from the expected analytical solution and does not converge. This is because of the fact that the distribution $p_b(x)$ does not mimic the function around its local maxima in the given interval as seen from the histograms (5-7) and figure (1). Since the probability distribution function $p_c(x)$ is exactly the same as the original function $f(x)$ that needs to be integrated, it mimcs the function at all values and thus produce the results closest to the analytical result.