24-623 2015 HM5

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1 Problem 1

Integration is performed with the random sampling monte-carlo integration of the variables. Program is evaluated at different sample sizes and the averages are reported for an average of 5 runs. Plots are shown for the value of PI and the error estimates at different sample sizes in Figures. 1 and 2.

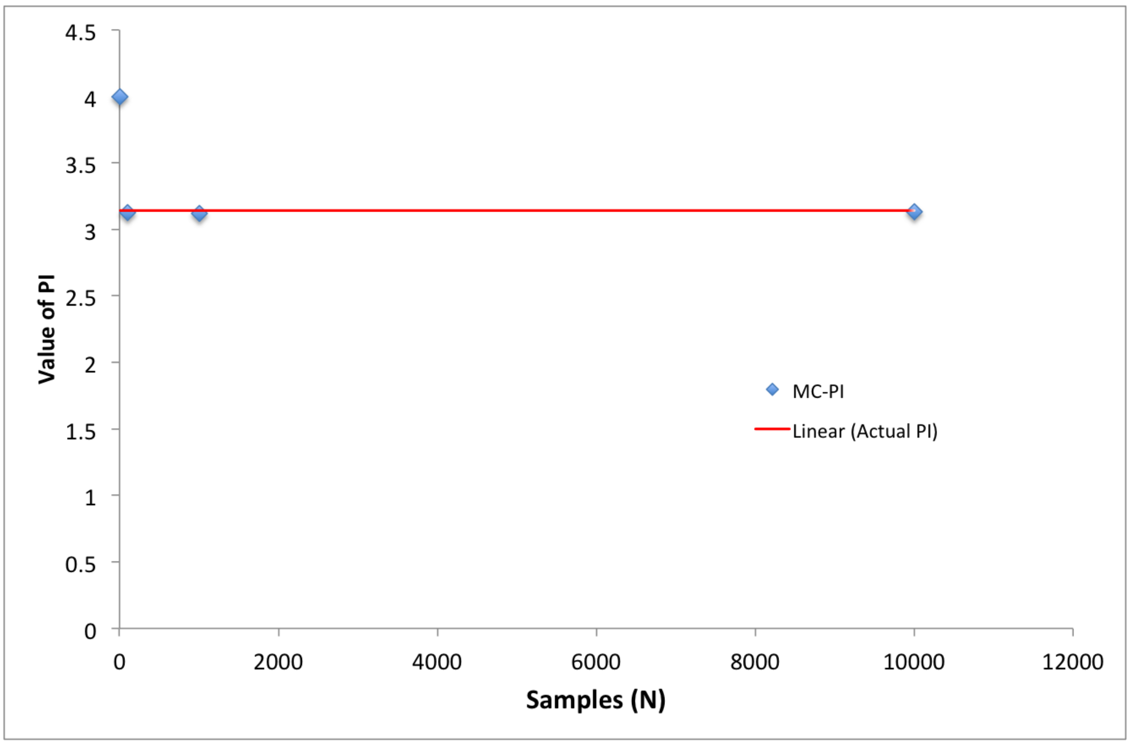

Figure 1: The figure shows the value of PI at different sample sizes computed from the random sampling monte-carlo integration.

The uncertainity for the computation of PI is estimated using relative error $(Q_N - \pi)/\pi$, where Q_N is the value of the PI obtained from the monte-carlo integration. The relative error is expected to change with the samples(N) according to the order, $O(1/\sqrt{N})$

The number of samples required for obtaining an accuracy till 20 significant digits is obtained from the relation

$$\frac{1}{\sqrt{N}} \propto \frac{Q_N - \pi}{\pi}$$

The absolute error will be in the order of 1.0e-21 for 20 significant digits accuracy.

$$\frac{1}{\sqrt{N}} \propto \frac{1.0e-21}{3.142857......(20digits)} \tag{1}$$

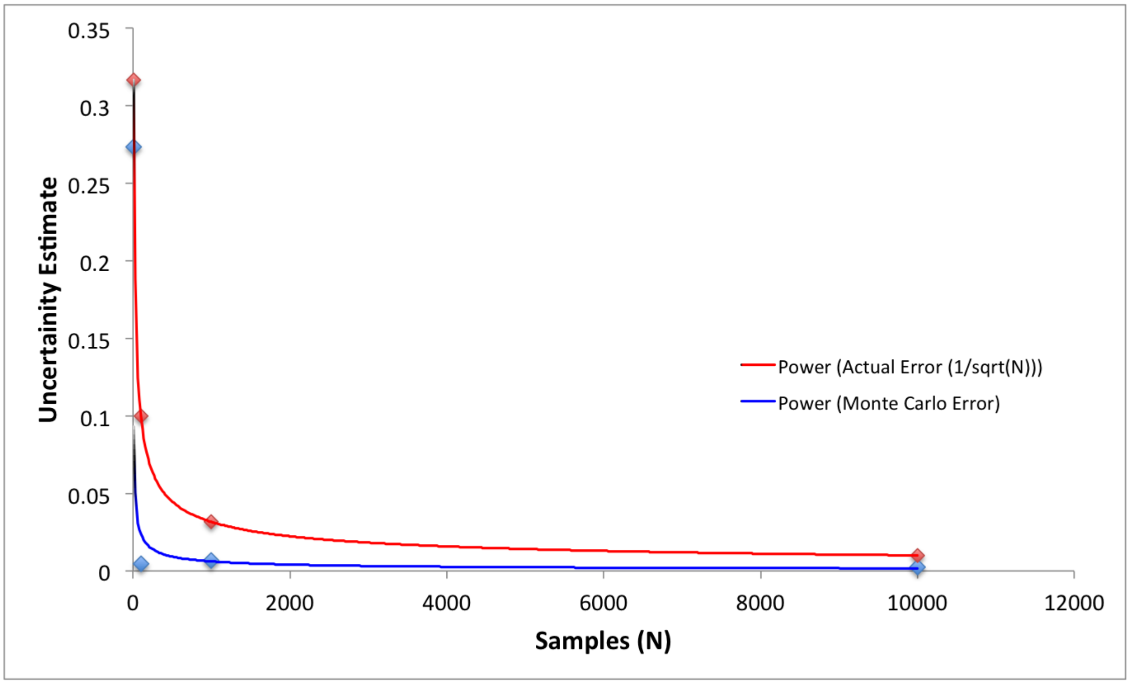

Figure 2: The figure shows the error estimates for the value of PI. The relative error is plotted against the sample sizes to show the convergence of the error with respect to the sample sizes. The actual error estimate varies according to the red curve.

$$N \propto \frac{1}{(3.18309e-22)^2} \tag{2}$$

Hence to achieve an accuracy of 20 significant digits from the Monte Carlo integration one would require, N = 1.0e+43 samples, computed from Eq.1.

2 Problem 2

2.1 a)

The values of $\langle U \rangle, \langle x \rangle, \langle x^2 \rangle$ are computed analytically and they are reported for harmonic oscillator a) $U(x) = x^2/2$.

$$\langle U \rangle = \frac{\int_{-\infty}^{\infty} U(x) exp(-\beta U(x))}{\int_{-\infty}^{\infty} exp(-\beta U(x))} \tag{3}$$

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x exp(-\beta U(x))}{\int_{-\infty}^{\infty} exp(-\beta U(x))} \tag{4}$$

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} x^2 exp(-\beta U(x))}{\int_{-\infty}^{\infty} exp(-\beta U(x))} \tag{5}$$

The average values are shown below :

Using the Metropolis Monte Carlo technique, the percentage of acceptance with respect to the values of β at different maximum step sizes is tabulated below 5 :

PARAMTERS : By looking at the Figs. 3, 4, 5, 6, the number of moves considered for this study is at 100,000. Better statistics could probably be obtained by using larger number of trail moves. The most

Table 1: Values of $\langle U \rangle, \langle x \rangle, \langle x^2 \rangle, aretabulatedbelowcomputedfromanalyticalexpressions.$

β	$\langle U \rangle$	$\langle x \rangle$	$\langle x^2 \rangle$
0.1	5	0.0	10
1	0.4998	0.0	1.0
5	0.1	0.0	0.2
10	0.05	0.0	0.1

Table 2: Percentage of acceptance of the moves with respect to various values of β and max. step sizes is shown below.

δ dx_{max}	β=0.1	β=1	β=5	β=10
0.05	50.024	49.544	49.025	48.543
0.5	48.491	44.948	39.232	34.891
5	35.184	15.809	7.152	5.097

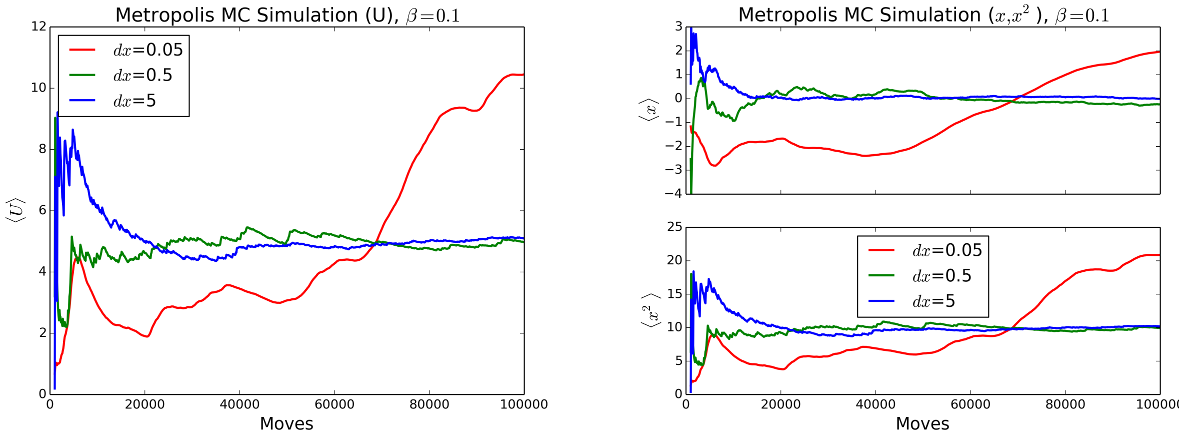

Figure 3: Monte Carlo Simulation of oscillator at $\beta = 0.1$

important factor considered in this case is the value of step size. Different step size values are considered for every value of β=0.1,1,5,10 and the best value of step size is chosen based on acceptance percentage of the moves as shown in Table. 5. At the maximum step size of 0.5, the average value of the parameters oscillate about the standard value. Hence, a maximum step size of 0.5 is considered for data analysis. The following plots (Figs. 3, 4, 5, 6) gives the information. Running averages are plotted in Figs. 3, 4, 5, 6.

2.2 b)

The values of $\langle U \rangle, \langle x \rangle, \langle x^2 \rangle$ are computed analytically for oscillator b) $U(x) = x^4 - 2x^2 + 1$. The average values are computed using Eqns. 3, 4, 5

The average values are shown below in Table. 3:

Using the Metropolis Monte Carlo technique, the percentage of acceptance with respect to the values of β at different maximum step sizes is tabulated below 5. Running average of the parameters are also shown below in Figs. 7, 8, 9, 10

3 Bonus

Monte Carlo computations are performed with Kawasaki dynamics and an interesting feature is observed for the percentage of accepted moves. It is observed that the accpetance percentage of the moves increases when compared to the metropolis monte carlo.

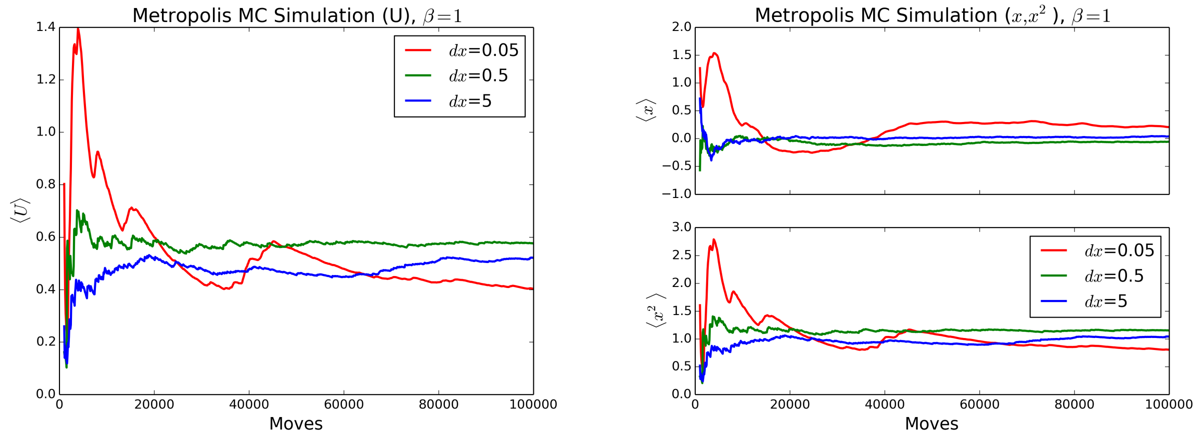

Figure 4: Monte Carlo Simulation of oscillator at $\beta = 1$

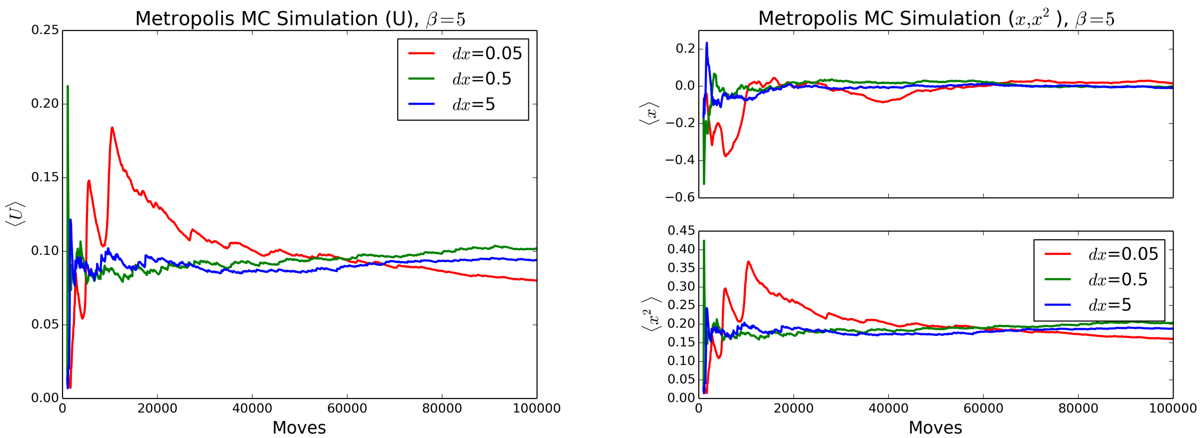

Figure 5: Monte Carlo Simulation of oscillator at $\beta = 5$

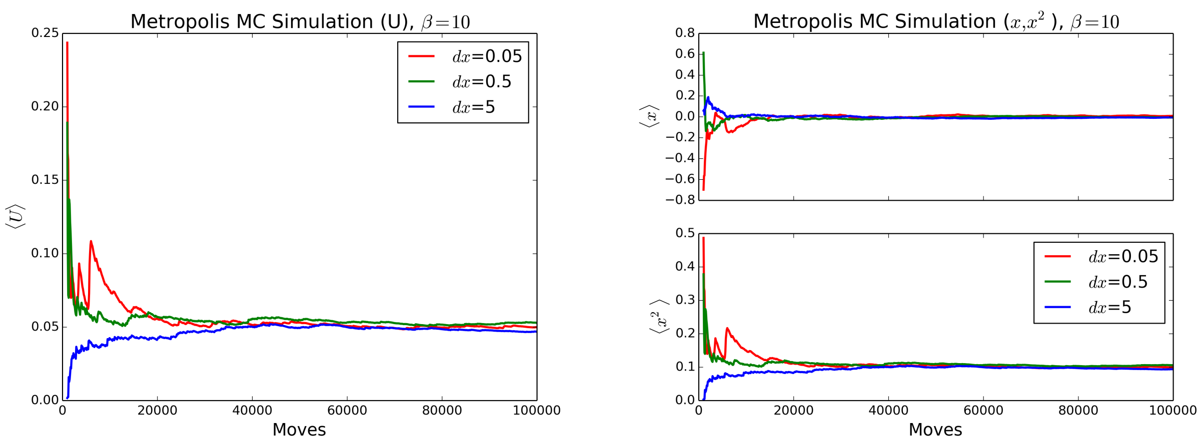

Figure 6: Monte Carlo Simulation of oscillator at $\beta = 10$

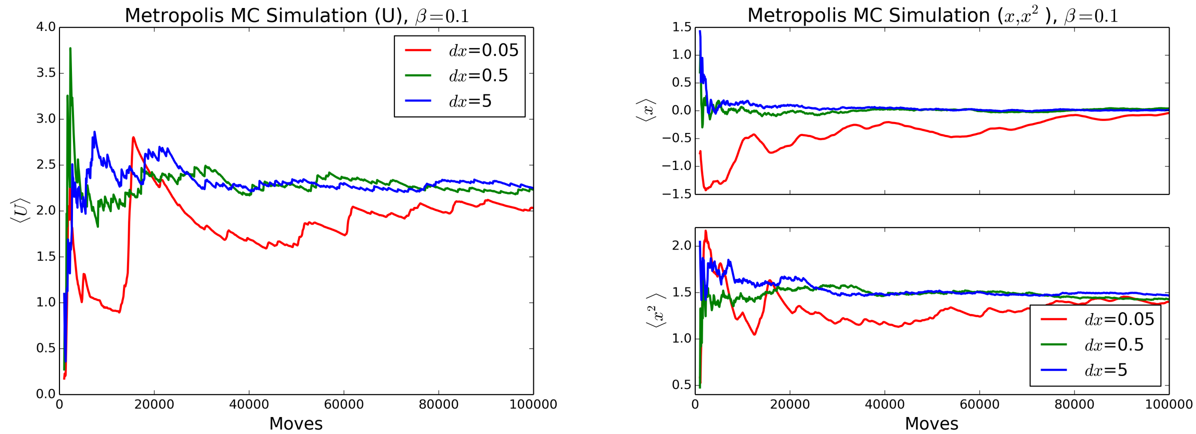

Figure 7: Monte Carlo Simulation of oscillator at $\beta = 0.1$

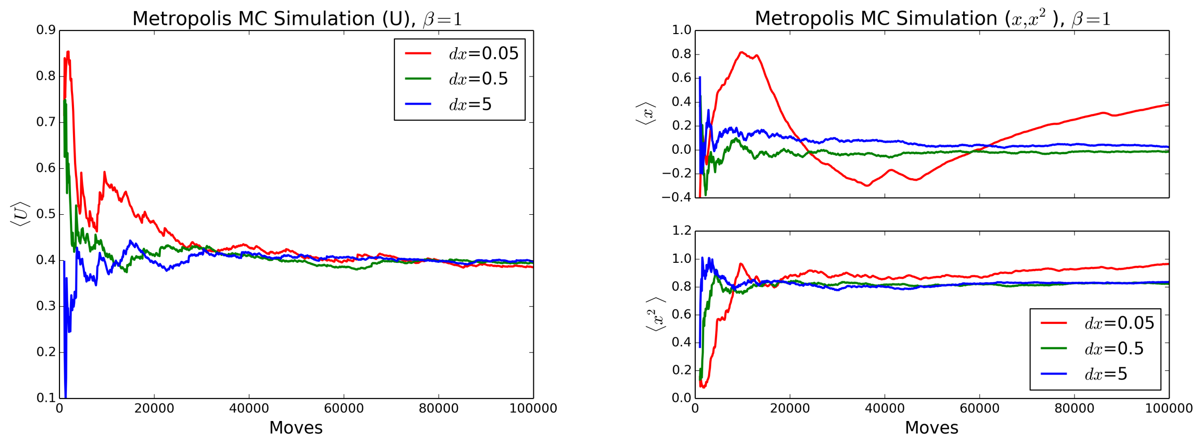

Figure 8: Monte Carlo Simulation of oscillator at $\beta = 1$

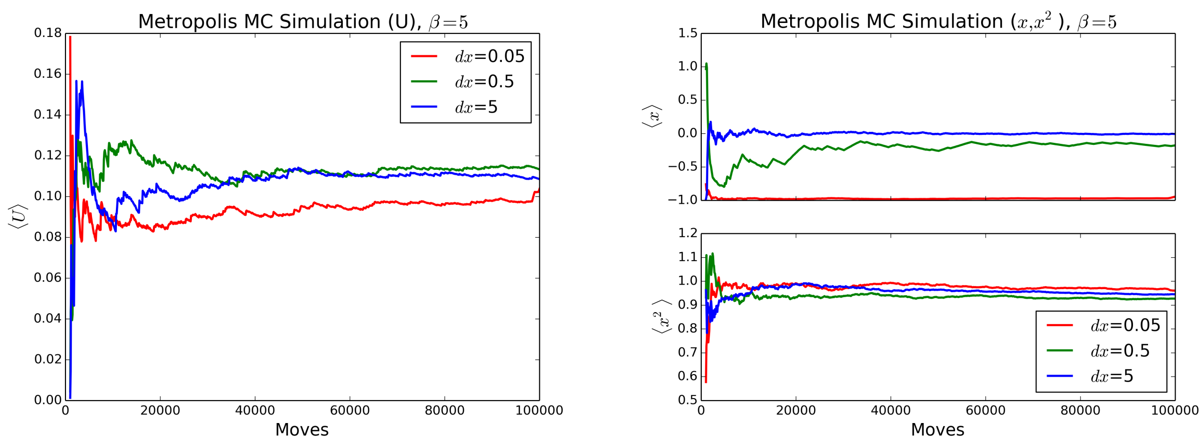

Figure 9: Monte Carlo Simulation of oscillator at $\beta = 5$

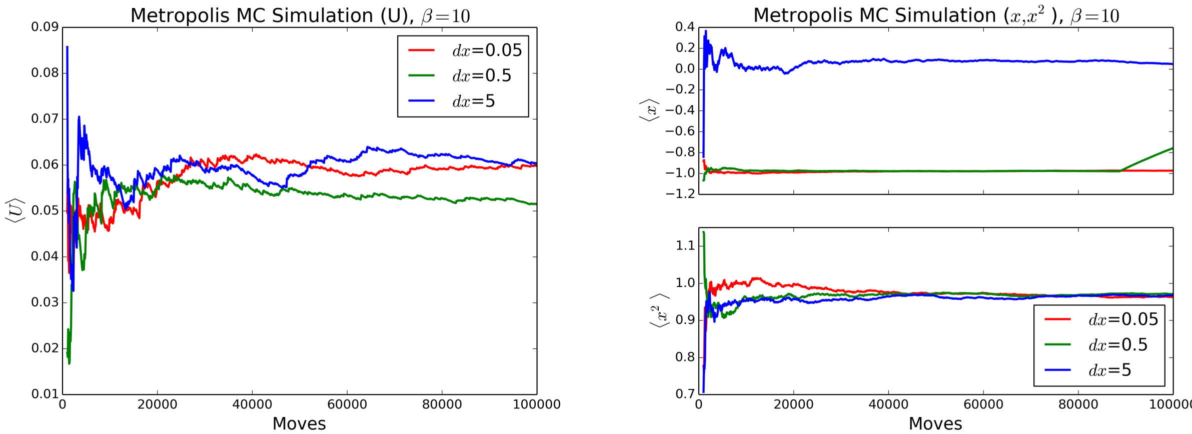

Figure 10: Monte Carlo Simulation of oscillator at $\beta = 10$

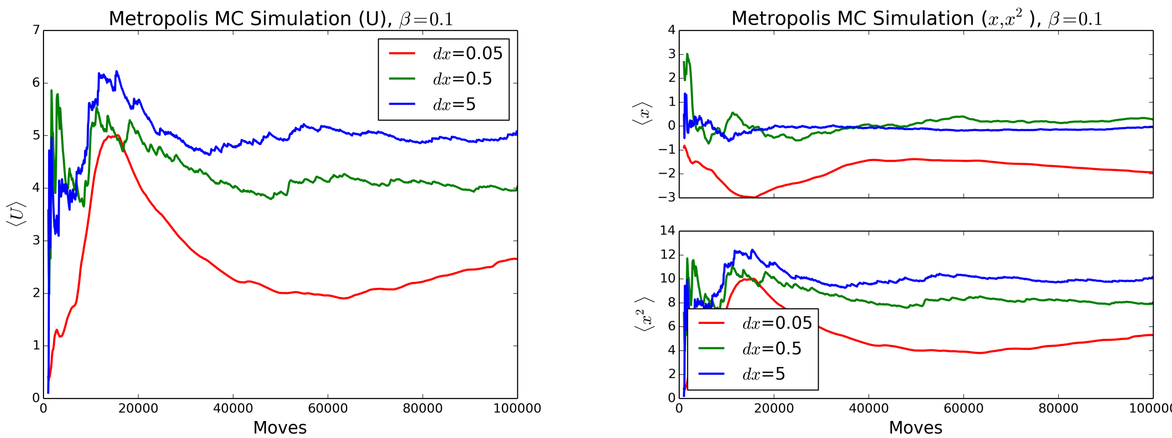

Figure 11: Monte Carlo Simulation of oscillator at $\beta = 0.1$

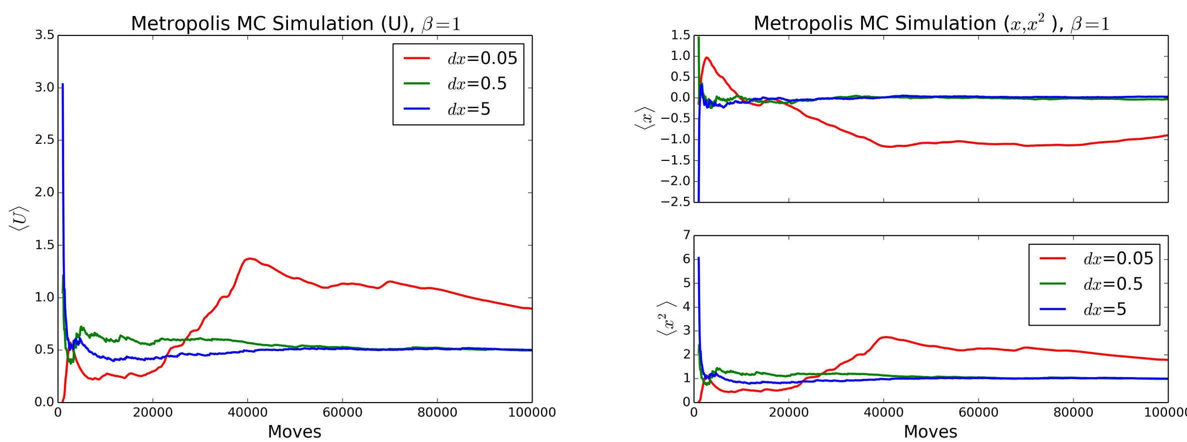

Figure 12: Monte Carlo Simulation of oscillator at $\beta = 1$

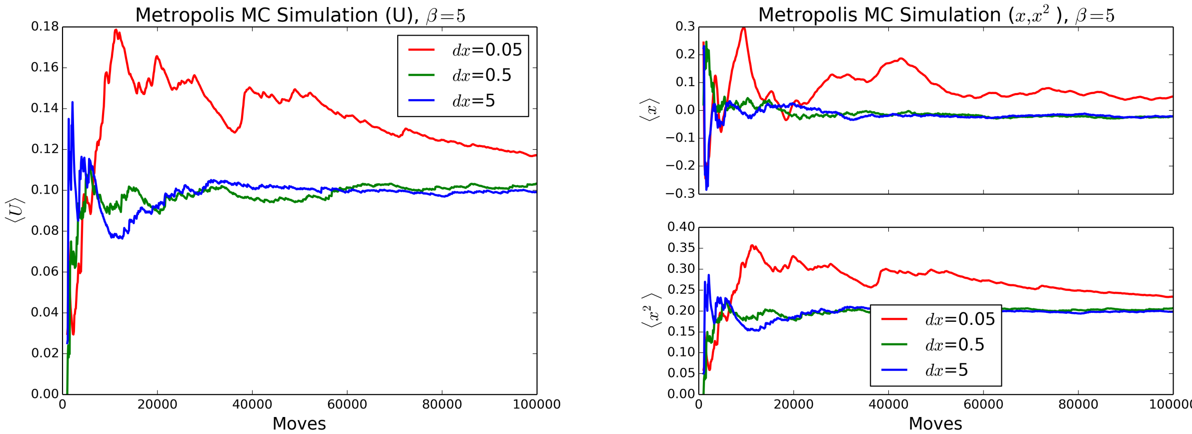

Figure 13: Monte Carlo Simulation of oscillator at $\beta = 5$

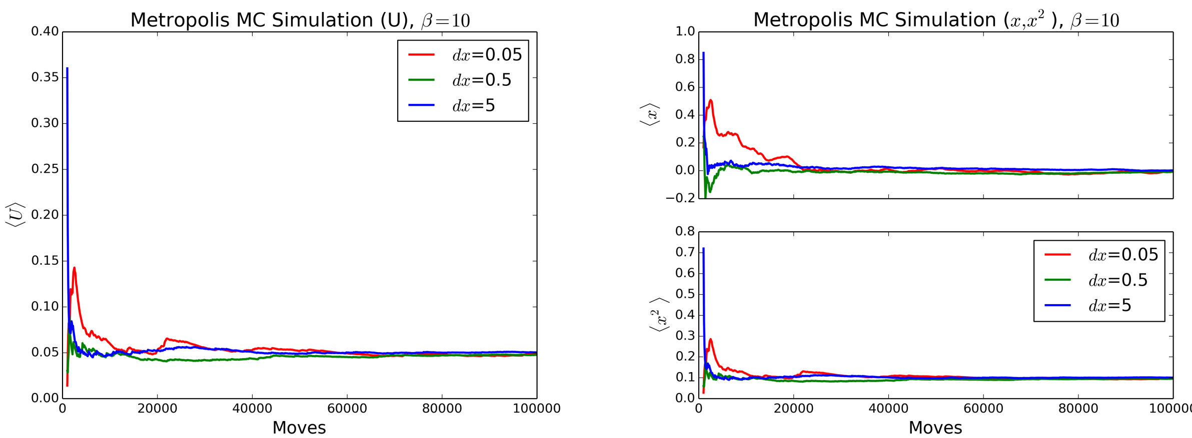

Figure 14: Monte Carlo Simulation of oscillator at $\beta = 10$

Table 3: Values of $\langle U\rangle, \langle x\rangle, \langle x^2\ \rangle aretabulatedbelowcomputedfromanalyticalexpressions.$

β	$\langle U\rangle$	$\langle x\rangle$	$\langle x^2\ \rangle$
0.1	2.1041757932	0.0	1.3958242068
1	0.417254512872	0.0	0.832745487128
5	0.113166059588	0.0	0.936833940412
10	0.0524772417986	0.0	0.972522758201

Table 4: Percentage of acceptance of the moves with respect to various values of β and max. step sizes is shown below.

δ $\mathrm{dx_{max}}$	β=0.1	β=1	β=5	β=10
0.05	49.722	48.696	46.986	45.614
0.5	46.299	40.189	25.116	18.07
5	19.853	12.223	5.476	3.931

3.1 Detailed Balance

For the detailed balance to obey, the rate to come to the 'new' configuration from 'old' configuration equals to that of from 'old' configuration to 'new' configuration.

$$p_{new}P(old \to new) = p_{old}P(new \to old) \tag{6}$$

Lets say that $P(old \to new)$ can be written as $acc(old \to new)\alpha(old \to new)$, hence

$$\frac{acc(old \to new)\alpha(old \to new)}{acc(new \to old)\alpha(new \to old)} = \frac{P(new)}{P(old)} \tag{7}$$

Hence the accpetance probability condition from old configuration to new configuration can be written as,

$$acc(old \to new) = \frac{P(new)}{P(old)}\frac{\alpha(new \to old)}{\alpha(old \to new)}acc(new \to old) \tag{8}$$

This would give us the acceptance probability to go from old state to new state as follows :

$$\boxed{acc(old \to new) = \frac{exp(-\beta\delta E/2)}{exp(-\beta\delta E/2) + exp(\beta\delta E/2)}acc(new \to old)} \tag{9}$$

By exploring the acceptance probability from new state to old state would give us :

$$\boxed{acc(new \to old) = \frac{exp(\beta\delta E/2)}{exp(\beta\delta E/2) + exp(-\beta\delta E/2)}acc(old \to new)} \tag{10}$$

where, $\delta E = U(new) - U(old)$, which takes a negative sign in vice-versa.

Table 5: Percentage of acceptance of the moves with respect to various values of β and max. step sizes is shown below.

δ $\mathrm{dx_{max}}$	β=0.1	β=1	β=5	β=10
0.05	50.231	50.205	49.819	50.168
0.5	50.194	48.93	45.499	42.05
5	42.103	20.209	9.138	6.509