TUM
Algorithms for UQ
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Exercise 1: Monte Carlo Sampling and Variation Reduction Techniques

Group 6

1 Introduction to Monte Carlo sampling estimator

Assignment 1.1

We computed mean and variance of the exam scores G using numpy and Python functionalities. The mean value was identical with both methods, $\mu = 1.647058$. This is due to the fact that the mean estimator is unbiased. The variance computed with Python functionality was $\sigma_P^2 = 0.148897$, whereas numpy function was $\sigma_{np}^2 = 0.140138$. This was due to the bias of the variance estimator; when multiplying by $\frac{1}{N}$ the variance estimator contains bias, however, when the factor is corrected to $\frac{1}{N-1}$, using numpy's variance functionality with ddof = 1, we had $\sigma_{np}^2 = \sigma_P^2$.

Assignment 1.2

We consider a bivariate normally distributed random variable X with mean $\mu = [-0.4, 1.1]^T$ and covariance matrix $V = [[2, 0.4], [0.4, 1]]$. In Table 1, for each sample size, we report the first component of the mean estimation and two estimated covariance values.

Sample Size	**Mean (1st Component)**	**Covariance (V_{00})**	**Covariance (V_{01})**
10	-0.5811	1.6687	-0.1651
100	-0.2211	2.0315	0.6643
1000	-0.4293	2.0002	0.4221
10000	-0.4031	2.0028	0.4052

Table 1: Sample mean and covariance entries for increasing sample sizes.

Remark. The covariance matrix V is symmetric, giving $V_{01} = V_{10}$.

Since we know the true values of our mean and covariance, we can plot the absolute error. We also include a graph showing the RMSE for the mean estimator.

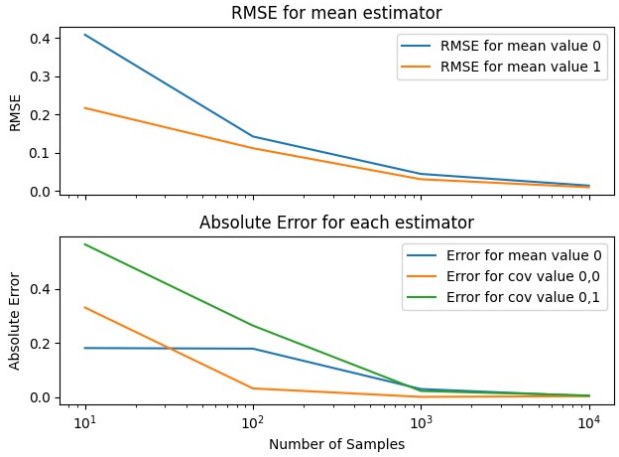

Figure 1: RMSE and absolute error for varying sample sizes.

The analytical derivation gives that the error decreases with $N^{-\frac{1}{2}}$, where N is the number of samples. Using the log-log plot as above, this corresponds to a straight line on the graph, meaning we achieved the expected results.

To estimate the error of the covariance matrix, however, we cannot directly use the same formula for RMSE. The formula for the RMSE of the mean is given by

$$\sqrt{\mathbb{E}\left[\|\hat{\mu} - \mu\|^2\right]}$$

and only contains scalar valued entries. In order to use a similar formula for the matrix estimation, we have to introduce a matrix norm, for example the Frobenius norm. In this case, we can define the MSE of the covariance estimator as $MSE = \mathbb{E}\left[\|\hat{V} - V\|_F^2\right]$. For further reading we refer to Letac and Massam - All invariant moments of the Wishart distribution, and Gupta and Nagar, Matrix Variate Distributions, 2000.

2 Monte Carlo integration

The second assignment was concerned with approximation of integrals of real-valued functions on finite intervals using Monte Carlo methods. An integral $I = \int_a^b f(x)\,dx$ can be computed using probabilistic techniques as

$$I = \mathbb{E}\left[f(x)\right] = \int_a^b f(x)\rho(x)\,dx, \tag{1}$$

with ρ being the density function of the uniform distribution $\mathcal{U}(a, b)$.

Assignment 2.1

We estimated $F = \int_0^1 \sin(x)\,dx$. In this case $\rho(x) = 1$ on $[0, 1]$, and we can use the Monte Carlo estimator

$$F \approx \hat{F}_f = \frac{1}{N} \sum_{i=1}^{N} f(x_i), \tag{2}$$

where we sample $\{x_i\}_{i=1}^N$ from $\mathcal{U}(0, 1)$.

The integral can also be computed analytically: $F = \cos(0) - \cos(1) = 1 - \cos(1)$, and we compare this result with our approximation.

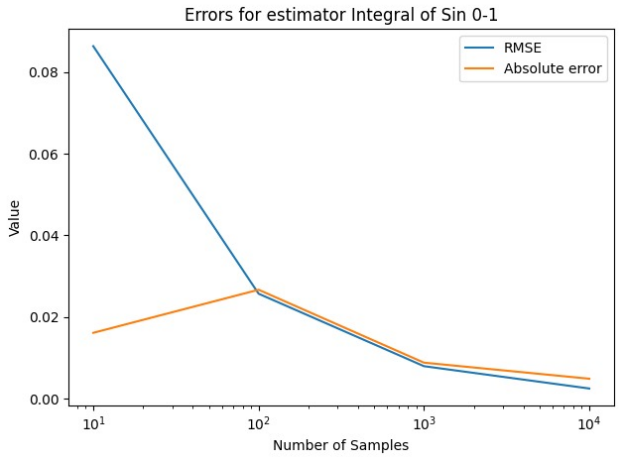

Figure 2: RMSE vs. exact error for sin estimator.

The absolute error is $\epsilon = |F - \hat{F}|$ and for the RMSE we use the formula from Assignment 1.1. Using the log-log plot as above and considering the convergence of order $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$ for RMSE, we conclude our model behaves as expected. The error decreases with increasing number of samples.

Assignment 2.2

We estimated $F = \int_2^4 \sin(x)\,dx$ in two different ways. The main difference from before is that now $\rho(x) = \frac{1}{2}$ on $[2, 4]$ and our integral is

$$\mathbb{E}\left[\sin(x)\right] = \int_2^4 \sin(x)\frac{1}{2}\,dx.$$

Draw samples from $\mathcal{U}(2, 4)$

We can rewrite the above relation as

$$2 \cdot \mathbb{E}\left[\sin(x)\right] = \int_2^4 \sin(x)\,dx, \tag{3}$$

directly draw samples from $\mathcal{U}(2,4)$ and use a modified version of the Monte Carlo estimator

$$F \approx \hat{F}_f = \frac{2}{N}\sum_{i=1}^{N} f(x_i).$$

Draw samples from $\mathcal{U}(0,1)$ and apply linear transformation

We keep in mind the PDF is now $\rho(x) = \frac{1}{2}$. We have

$$\int_2^4 \sin(x)\frac{1}{2}\,dx = \int_0^1 2\sin(2(t+1))\,dt,$$

where we used a change of variables $x = 2(t+1)$ in order to translate the interval of integration to $[0,1]$.

We can now use the original Monte Carlo technique

$$F \approx \hat{F}_f = \frac{1}{N}\sum_{i=1}^{N} f(x_i),$$

with $f(x) = 2\sin(2x+2)$ and $\{x_i\}_{i=1}^N$ from $\mathcal{U}(0,1)$.

Remark. In our solution we applied a linear transformation (change of variables) in the integral. Another approach is to draw samples from $\mathcal{U}(0,1)$ and apply a linear transformation on the samples:

$$x \mapsto \frac{(4-2)(x-0)}{1-0} + 2 = 2x + 2$$

and then use equation (3) on the transformed samples.

Again, we can compute the integral analytically and compare the errors.

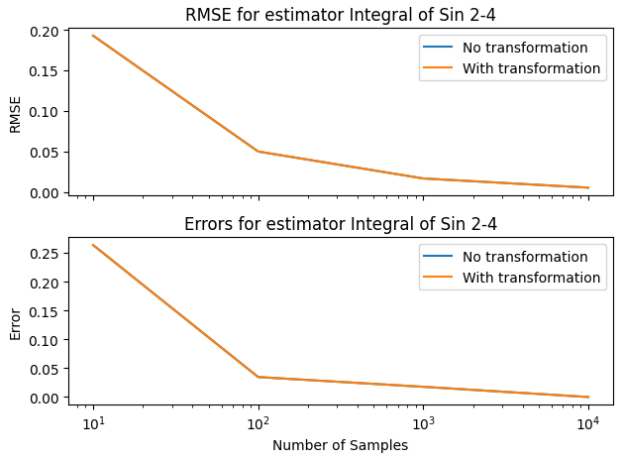

Figure 3: RMSE and exact error for sine estimator.

Remark. Both methods produced the same RMSE and absolute error, so the error values in Figure

3 overlap.

Note, the RMSE and standard error decrease as the number of samples increases. Since we only had to modify the sampling method, the RMSE has the same interpretation in Assignment 2.1 and 2.2.

3 Improving standard Monte Carlo sampling

Assignment 3

For this part, we estimated $I = \int_0^1 f(x)\,dx$ with $f(x) = e^x$ in three variations of the Monte Carlo method. Again we used $N = [10, 100, 1000, 10000]$ samples for each method. We can compute the integral analytically,

$$\int_0^1 e^x\,dx = e^1 - e^0 = e - 1 \approx 1.71828,$$

and we will compare the analytical value with each approximation method.

Standard Monte Carlo sampling

First we used the standard Monte Carlo estimator, given in Equation (2).

Sample Size	Absolute Error	Var of MC estimator
10	0.09863603	0.0225587
100	0.04515856	0.0024708
1000	0.00359471	0.0002415
10000	0.00370581	2.427e-05

Table 2: Monte Carlo absolute error and variance for increasing sample sizes.

From Table 2, we observe that the absolute error of the Monte Carlo estimator decreases as the sample size increases, as expected. The most significant improvement occurs between $N = 100$ and $N = 1000$, while the error change from $N = 1000$ to $N = 10000$ is marginal, indicating diminishing returns at larger sample sizes.

The variance of the Monte Carlo estimator decreases approximately at the expected rate of $\mathcal{O}\left(\frac{1}{N}\right)$. We can see this by computing the product $N \cdot \mathrm{Var}(\hat{I})$ for various sample sizes:

$$\begin{aligned}
N = 10 \quad &\Rightarrow \quad N \cdot \mathrm{Var}(\hat{I}) = 0.2256 \\
N = 100 \quad &\Rightarrow \quad N \cdot \mathrm{Var}(\hat{I}) = 0.2471 \\
N = 1000 \quad &\Rightarrow \quad N \cdot \mathrm{Var}(\hat{I}) = 0.2416 \\
N = 10000 \quad &\Rightarrow \quad N \cdot \mathrm{Var}(\hat{I}) = 0.2427
\end{aligned}$$

Since these values remain approximately constant, the data supports $\mathrm{Var}(\hat{I}) \propto \frac{1}{N}$. In general, increasing the sample size improves accuracy but with a decrease in efficiency as $N \to \infty$.

Control Variates

Next we used the control variates method with three different auxiliary functions:

$$\phi_1(x) = x,\ \phi_2(x) = 1 + x,\ \phi_3(x) = 1 + x + \frac{x^2}{2},$$

with known expected value. The unbiased estimator of the control variates is given by

$$I_{CV} = \hat{I}_f + \alpha\,(\mathbb{E}[\phi_i(x)] - \hat{I}_{\phi_i}), \tag{4}$$

where $\hat{I}_f$ is the Monte Carlo estimator of $f(x) = e^x$, α is the control variates parameter and $\hat{I}_{\phi_i}$ is the Monte Carlo estimator of $\phi_i(x)$ for each $i \in \{1, 2, 3\}$. We computed I_{CV} for each ϕ_i.

For each $i \in \{1, 2, 3\}$, we computed $\mathbb{E}[\phi_i(x)]$:

$$\mathbb{E}[\phi_1(x)] = \frac{1}{2},\ \mathbb{E}[\phi_2(x)] = \frac{3}{2},\ \mathbb{E}[\phi_3(x)] = \frac{5}{3}.$$

In Tutorial 4, Task 3, we showed that

$$\mathrm{Var}(I_{CV}) = \frac{\sigma_f^2}{N} + \alpha^2\frac{\sigma_{\phi_i}^2}{N} - 2\alpha\frac{\rho_{f\phi_i}\sigma_f\sigma_{\phi_i}}{N}, \tag{5}$$

where $\rho_{f\phi_i} = \frac{\mathrm{Cov}(f(x),\phi_i(x))}{\sigma_f\sigma_{\phi_i}}$ is the Pearson correlation coefficient between f and ϕ_i. In addition, we showed that the value of α which minimizes $\mathrm{Var}(I_{CV})$ is given by

$$\alpha_{\phi_i}^* = \frac{\rho_{f\phi_i}\sigma_f}{\sigma_{\phi_i}} \approx \frac{\hat{\rho}_{f\phi_i}\hat{\sigma}_f}{\sigma_{\phi_i}},$$

which we used in Equation (4) to compute the control variates estimates. In Tables 3-5 below, we give the absolute error of the estimate for each ϕ_i, the variance of the estimator and the optimal α^* values.

Among the three auxiliary functions tested, the function $\phi_3(x) = 1 + x + \frac{x^2}{2}$ yielded the best performance. This is because it closely approximates the target function $f(x) = e^x$ via its Taylor expansion, leading to a higher correlation with $f(x)$ and consequently a greater reduction in variance. The results demonstrate that the control variates method using an auxiliary function with has high correlation with $f(x)$ is effective, even for small sample sizes.

Sample Size	**Abs. Error**	**Var(I_{CV})**	**$\alpha_{\phi_1}^*$ approx**
10	2.575e-03	1.085e-06	1.701
100	3.887e-03	1.609e-07	1.632
1000	1.179e-03	1.721e-08	1.675
10000	3.776e-04	1.634e-09	1.694

Table 3: Estimator Performance for ϕ_1

Sample Size	Abs. Error	$\mathbf{Var}(I_{CV})$	$\alpha^*_{\phi_2}$ approx
10	2.575e-03	1.085e-06	1.716
100	3.887e-03	1.609e-07	1.632
1000	1.179e-03	1.721e-08	1.675
10000	3.776e-04	1.634e-09	1.694

Table 4: Estimator Performance for ϕ_2

Sample Size	Abs. Error	$\mathbf{Var}(I_{CV})$	$\alpha^*_{\phi_3}$ approx
10	1.719e-03	3.186e-08	1.136
100	1.965e-03	3.436e-09	1.092
1000	4.056e-04	2.288e-10	1.121
10000	7.638e-05	2.128e-11	1.133

Table 5: Estimator Performance for ϕ_3

Importance Sampling

Instead of drawing from a uniform distribution, we have samples from a different distribution $q(x)$. This approach is particularly useful when the integrand $f(x)p(x)$ is concentrated in regions that are poorly represented by uniform sampling. The key idea is to select a sampling distribution $q(x)$ that is more "aligned" with the shape of the function being integrated to reduce estimation error.

In our case the proposed distributions were Beta distributions with parameters $(\alpha_1, \beta_1) = (5, 1)$ and $(\alpha_2, \beta_2) = (0.5, 0.5)$. As we can see in the table shown below, the absolute error for Beta$(5, 1)$ does not significantly drop with increasing number of sample, and stays on the same order of magnitude. The problem with this proposed distribution is that it draws samples very close to 1, since its PDF is of the form $x \mapsto B(5, 1)x^4$.

The better choice of parameters is Beta$(0.5, 0.5)$, which more evenly draws samples from $[0, 1]$.

Sample Size	Abs Error (Beta(5,1))	Abs Error (Beta(0.5,0.5))
10	0.74452936	0.42739650
100	0.43929634	0.03346826
1000	0.24634799	0.02163726
10000	0.19246763	0.00438205

Table 6: Absolute errors of importance sampling estimates using Beta(5,1) and Beta(0.5,0.5).

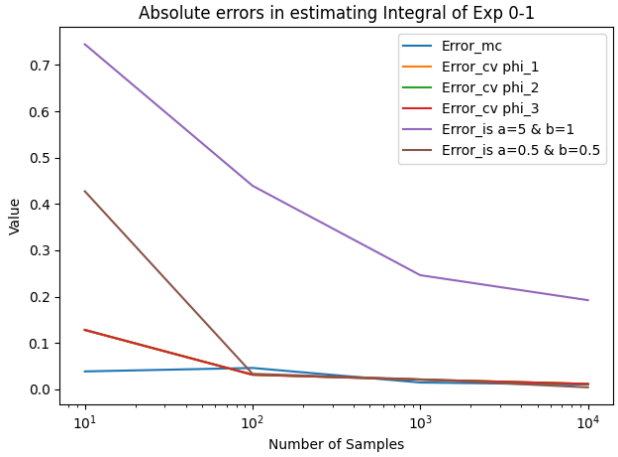

Figure 4: Absolute errors for different methods to estimate $f(x) = e^x$.

Figure 4 compares the absolute errors of various integration methods for estimating $\int_0^1 e^x \, dx$. The control variates based on $\phi_1(x) = x$ and $\phi_2(x) = 1 + x$ perform identically, showing that adding a linear combination of an auxiliary function does not affect the variance reduction. While standard Monte Carlo estimation outperforms the other methods for small N, the control variates and importance sampling methods (with $\alpha = \beta = 0.5$) becomes more accurate as the sample size grows.

4 Monte Carlo sampling for forward propagation

In this assignment, we study uncertainty propagation in a second-order linear damped oscillator model governed by the system of differential equations:

$$\begin{cases} \frac{d^2y(t)}{dt^2} + c\frac{dy(t)}{dt} + ky(t) = f\cos(\omega t), \\ y(0) = y_0, \\ \frac{dy}{dt}(0) = y_1, \end{cases}$$

where c, k, and f denote the damping coefficient, spring constant, and forcing amplitude, respectively. The parameter ω is the frequency, and y_0, y_1 are the initial conditions.

We assume that ω is uncertain and distributed uniformly as $\omega \sim \mathcal{U}(0.95, 1.05)$. We propagate the uncertainty through the system by sampling values of ω and solving the ODE numerically for each realization.

Two methods are used to perform this analysis:

- Standard Monte Carlo sampling,
- Quasi-Monte Carlo sampling using Halton sequences.

For both approaches, we compute the sample mean and variance of $y(10)$ using $N = [10, 100, 1000, 10000]$

samples. These results are compared to a reference solution, which contains values computed with $N_{\text{ref}} = 10^6$ samples.

Additionally, we illustrate the effect of uncertainty by plotting ten trajectories of $y(t)$ over the interval $t \in [0, 10]$, each corresponding to a different sampled value of ω from the standard Monte Carlo method.

Sample size	**Mean**	**Abs Error (Mean)**	**Variance**	**Abs Error (Var)**
10	-0.438375	0.000562	0.000225	0.000028
100	-0.437420	0.001517	0.000217	0.000020
1000	-0.438408	0.000529	0.000204	0.000007
10000	-0.438926	0.000011	0.0001986	0.0000018

Table 7: Monte Carlo estimates of $\mathbb{E}[y(10)]$ and $\text{Var}[y(10)]$ compared to reference values.

Sample size	**Mean**	**Abs Error (Mean)**	**Variance**	**Abs Error (Var)**
10	-0.43833755	0.00059948	0.00022537	0.00002859
100	-0.43742012	0.00151691	0.00021715	0.00002037
1000	-0.43840757	0.00052946	0.00020410	0.00000732
10000	-0.43892632	0.00001071	0.00019863	0.00000185

Table 8: Estimation of $\mathbb{E}[y(10)]$ and $\text{Var}[y(10)]$ with the Halton sequences approach.

The results show that as the number of samples increases, both the estimated mean and variance of $y(10)$ converge toward the reference values. The absolute errors in both mean and variance decrease significantly with larger sample sizes, demonstrating the expected convergence behavior of the Monte Carlo method. The spike in relative error for the mean is due to the random generation of the samples.

We also observe that the approximations using uniform and Halton sequence based sampling are nearly identical. This is because, in one dimension, the Halton sequences generate deterministic evenly spaced samples across the target interval. As the sample size N increases, these samples closely resemble those obtained through uniform stochastic sampling, leading to similar approximation results.

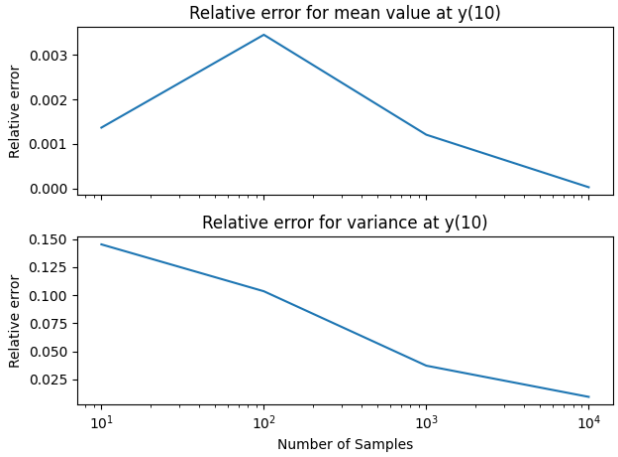

Figure 5: Visualization of relative error for mean and variance

Finally, we plot ten different trajectories for the sampled ω.

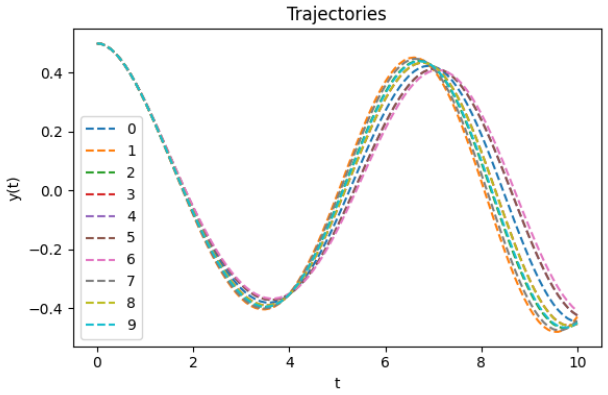

Figure 6: Trajectories of the oscillator for different frequencies ω