1 Exercise

In the first exercise we want to apply the QMC Methods to the first exercise of homework 1. We use the same idea as in HW1 to turn the calculation of an integral into a stochastic problem:

$$\begin{aligned}\int_{[0,1]^N} f(x)dx &= \int_{[0,1]^N} f(x)\cdot 1 dx \\ &= \int_{\mathcal{R}^N} f(x)p(x)dx \\ &= E(f(U)) \quad \checkmark\end{aligned}$$

Here $p(x)$ is the PDF of the uniform distibution over $[0,1]^N$ and U is a random variable sampled from this distribution.
This was all discussed already in the last homework. If we now look at the MC estimator, which we already introduced in the last homework:

$$\mathbb{E}[f(U)] \approx \sum_{m=1}^{M} \frac{1}{M} f(U_m) \quad \checkmark$$

where U_m are iid samples from the uniform distibution over $[0,1]^N$. This can also be seen as a quadrature formula with equal weights $\frac{1}{M}$, even though our samples are randomly distributed and not evenly distributed. Therefore we want to look at the idea of QMC, which uses points that are not randomly distributed, but instead ~~evenly distributed~~ in our domain. First we want to discuss how we will distribute the points in our domain. In the lecture, we saw, that the error, we get from the QMC method is depending on the discrepancy function of our points. This is defined as:

$$\Delta_p(x) = \hat{Vol}_p([0,x]) - Vol([0,x]) = \frac{1}{M}\sum_{m=1}^{M} \mathbf{1}_{[0,x]}(\xi_m) - \prod_{n=1}^{d} x_n \quad \checkmark$$

We can meassure the discrepancy of a pointset with regard to many different norms. One of the most prominently used norms for this is the $\mathcal{L}^\infty$-norm. We call the resulting value:

$$\Delta^\star_{P,N} := ||\Delta_P||_{\mathcal{L}^\infty([0,1]^N)} = \sup_{x\in[0,1]^N} |\Delta_p(x)| \quad \checkmark$$

the star discrepancy. There exist many different methods to generate points with small star discrepancy. The method we want to focus on during this homework are Sobol-points.
~~Even though plain QMC can give us a good estimate of the QoI, we want to find a hybrid between this method and MC.~~ This leads us to RQMC. This method generates a set of M (in our case Sobol-) points in $[0,1]^N$. Next we will generate s iid uniformaly distributed Samples U_j on the same set $[0,1]^N$. These will be used as shifts, that shift the sobol-points to new random locations. Therefore we get the QMC estimators:

$$I_{N,M}(f,\eta_n) = \frac{1}{M}\sum_{m=1}^{M} f(\xi_m + \eta_n)$$

Here we just have to pay attention, because our points could be shifted out of the domain $[0,1]^N$. Therefore we will use the lattice rule, meaning, that we actually use the points $(\xi_m + \eta_n) \mod 1$.

Now we want to take the s different QMC estimators and use standard MC on those. This gives us the following estimator:

$$I_{N,M}(f) = \frac{1}{sM} \sum_{n=1}^{s} \sum_{m=1}^{M} f(\xi_m + \eta_n)$$

Because we have ~~basicly~~ just used plain MC on the QMC estimators, the theoretical results, like CLT, still hold and we get the following RQMC-CLT-Boundary:

$$e_{N,M}(f) = \frac{c_0}{\sqrt{s}} \sqrt{\frac{1}{s-1} \sum_{n=1}^{s} (I_{N,M}(f, \eta_n) - I_{N,M}(f))^2}$$

In the following numerical experiments we looked at the same integrals as in HW01 and we tried to compare these results with the results we got from QMC. To make both experiments comparable, we had to assure, that the total amount of points, for which we calculate the funciton value, is the same for results, which we compare. We used 1000 starting samples and increased them by 500 samples until we reached a total of 100000 samples for the standard MC. For the QMC we always used 25 shifts. This means, if we want to get the same number of total points, that we have to divide the above numbers by 25. This gives us: 40 initial sobol-points, increments of 20 sobol-points and a final amount of 4000 sobol points.
~~Bellow~~, one can see the error and CLT comparisons between standard MC and RQMC. One can see, that the RQMC-CLT boundary is ~~allways~~ underneath the standard CLT boundary. This shows that we actually achieve variance reduction.
The only case, where RQMC performs worse than standard MC is the 20d version of the Corner Peak function.

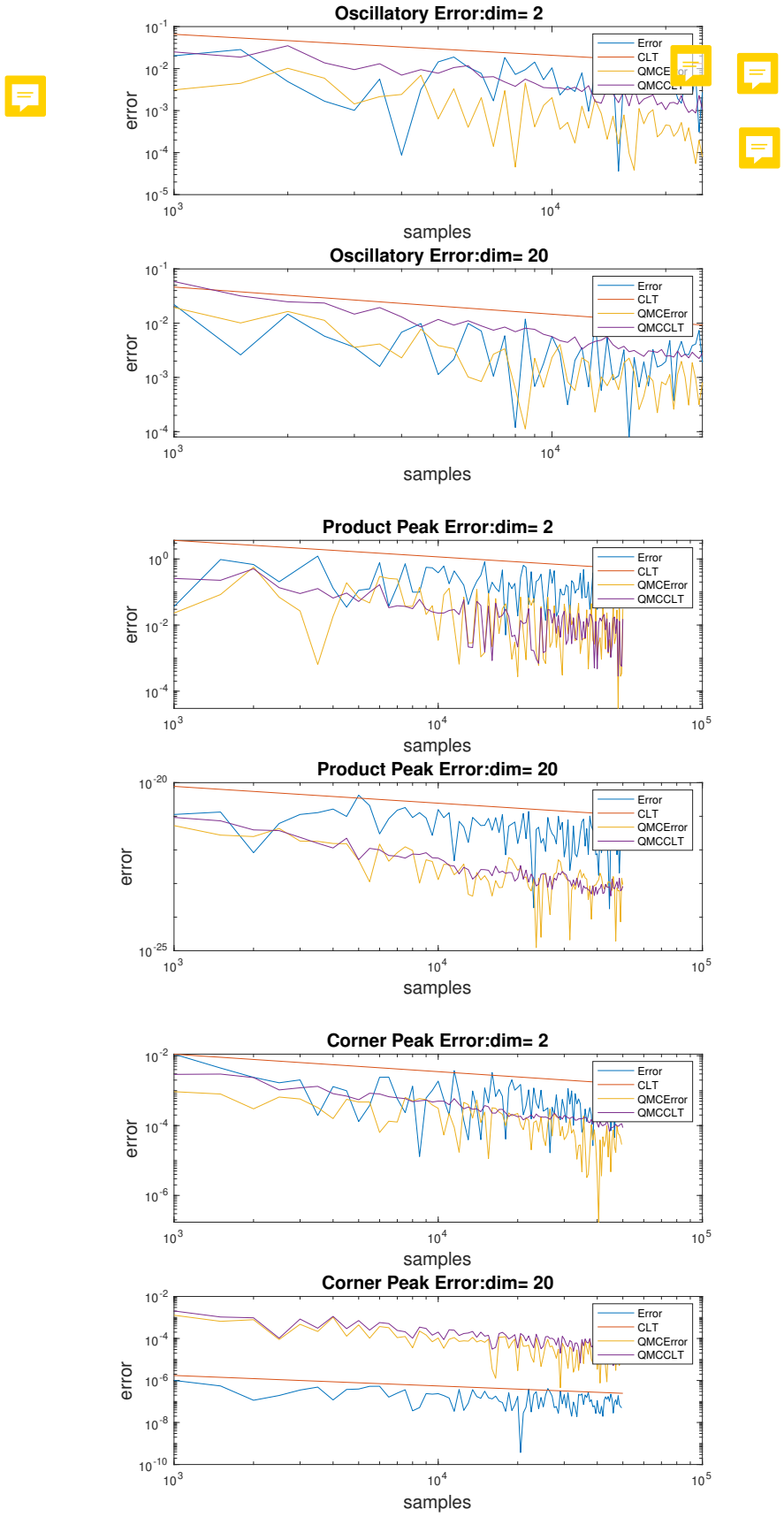

Figure 1: Error comparison for QMC and standard MC, each time showing the CLT Bounaries and the absolute error (Oscillatory, Product Peak and Corner Peak)

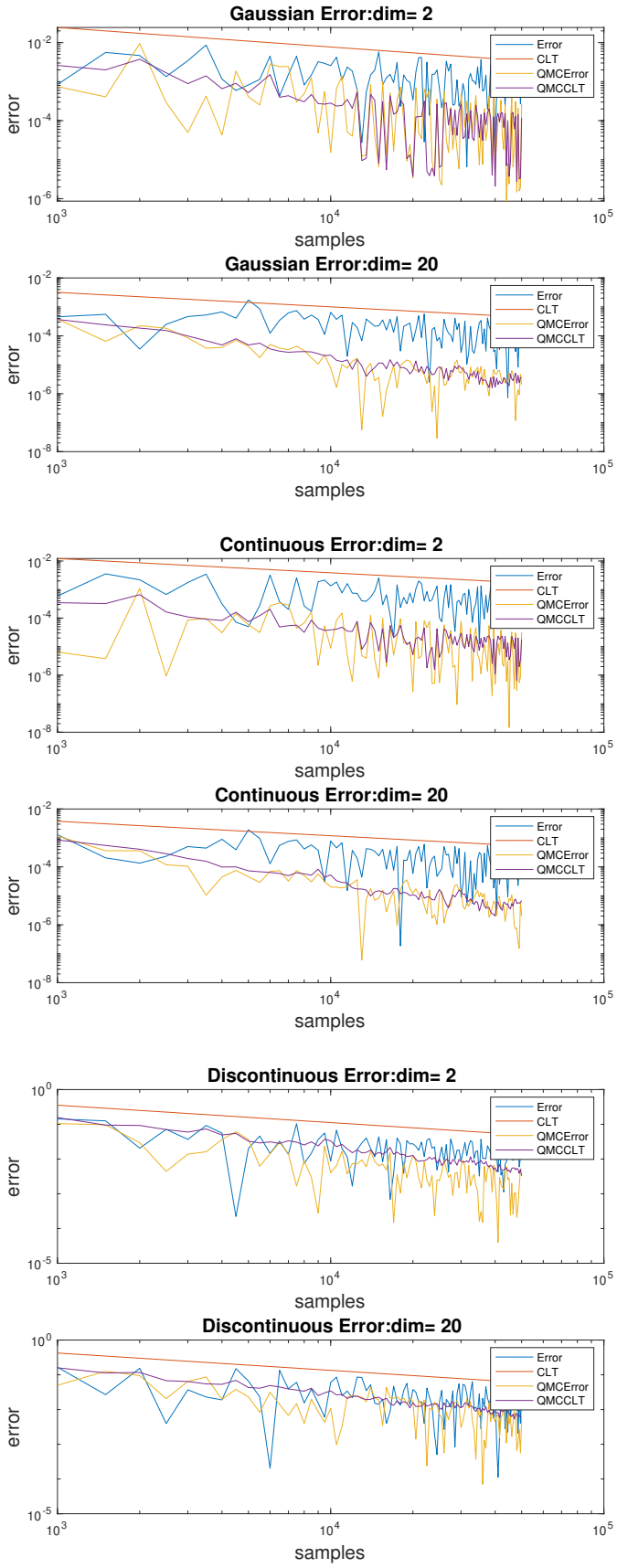

Figure 2: Error comparison for QMC and standard MC, each time showing the CLT Bounaries and the absolute error (Gaussian, Continuous and Discontinuous)

1.5.3

In this example we have to adjust some things from HW01. The use of QMC needs, that we sample from a uniform distribution on $[0,1]^N$. In HW01 we calculated this integral by looking at it as an expected value regarding the normal distribution:

$$\frac{1}{2\pi}\int_{\mathcal{R}^2} \max(e^{x_1}+e^{x_2}-K,0)e^{-0.5(x_1^2+x_2^2)}dx_1dx_2 = E[\max(e^{x_1}+e^{x_2}-K,0)]$$

Where x_1 and x_2 are iid normal distributed RV. This is a problem, because QMC is (as mentioned before) only feasible for uniform distributions on $[0,1]^N$. This can however be fixed by applying the inverse of the standard normal cdf to our sobol points (componentwise). Because the cdf $\Phi : \mathcal{R} \to (0,1)$ is bijective. This gives us a homeomorphism between ~~$\mathcal{R}^2$~~ and $[0,1]^2$. This basicly gives us a coordinate transformation which makes it possible to just apply this function to the shifted sobol points and then apply the RQMC method as usual. One can see in the bellow graphs that we actually achieved a smaller error and that the CLT Boundaries become smaller, if we apply IS in addition to RQMC.

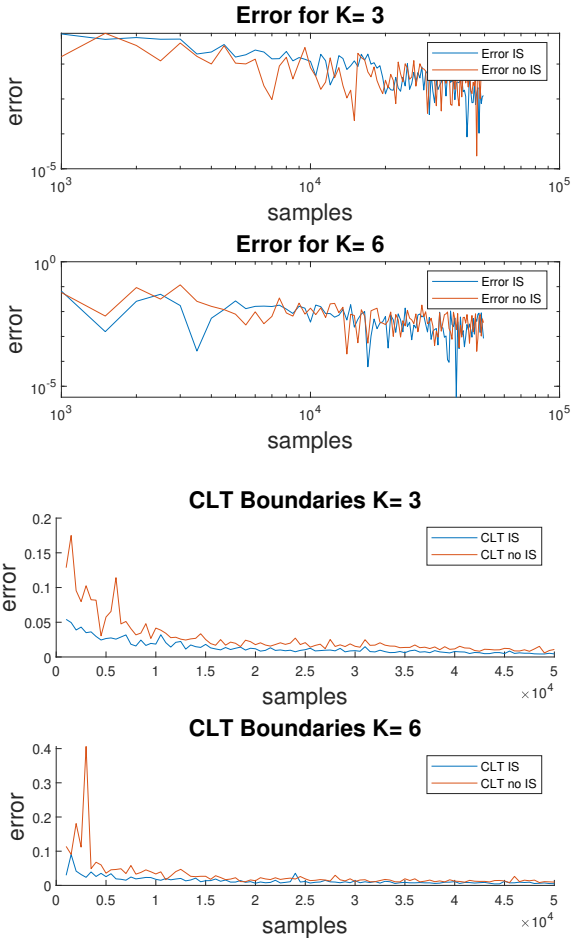

Figure 3: Error for the QMC Methods with and without Importance sampling, aswell as the CLT Boundaries

2 Exercise

2.5.1

We have the same PDE as in Homework 1, but we now want to apply RQMC, as define in Exercise 1. We utilize the Fourier expansion for the Lognormal Problem and use the same cutoff N as in Homework 1 to truance the sum

$$a(\omega, x) \approx \sum_{n=0}^{N} \kappa_n \left(y_n(\omega) \cos\left(\frac{n\pi x}{L_p}\right) + z_n(\omega) \cos\left(\frac{n\pi x}{L_p}\right)\right) \quad \checkmark$$

which means we choose, for $\nu \in \{2.5, \infty\}$, the cutoff $N \in \{19, 16\}$. To estimate the convergence we correlate the samples as follows

i) Generate M vectors $y_i \in \mathbb{R}^N$ and $z_i \in \mathbb{R}^N$ using $i4\_sobol\_generate(N, M, 0)$

ii) Shift each of these vectors y_i and z_i with independent normal vectors $\eta_{y,j}$, $\eta_{z,j} \in \mathbb{R}^N$

iii) Take a shifted vector from ii) and calculate $Q(u_{2h}(y_i, z_i, \eta_{y,j}, \eta_{z,j}))$ and $Q(u_h(y_i, z_i, \eta_{y,j}, \eta_{z,j}))$

iv) Repeat ii) S times and iii) M times, for a total of $S \cdot M$ different evaluations of $Q(u_{2h})$ and $Q(u_h)$

v) Approximate

$$E[Q(u_{2h})] \approx \frac{1}{SM} \sum_{j=1}^{S} \sum_{i=1}^{M} Q(u_{2h}(y_i, z_i, \eta_{y,j}, \eta_{z,j})) =: I_{N,M}(Q(u_{2h}))$$
$$E[Q(u_h)] \approx \frac{1}{SM} \sum_{j=1}^{S} \sum_{i=1}^{M} Q(u_h(y_i, z_i, \eta_{y,j}, \eta_{z,j})) = I_{N,M}(Q(u_h)) \quad \checkmark$$

with the independet samples from iv)

Similarly to exercise 1 we have the RQMC-CLT-Boundary

$$e_{N,M}(Q(u_h)) = \frac{c_0}{\sqrt{s}} \sqrt{\frac{1}{s-1} \sum_{n=1}^{s} (I_{N,M}(Q(u_h), \eta_n) - I_{N,M}(Q(u_h)))^2} \quad \checkmark$$

and the Bias error

$$e_{bias} = \frac{I_{N,M}(Q(u_h)) - E[Q(u)]}{E[Q(u)]} \approx \frac{1}{1 - 1/2^p} \frac{I_{N,M}(Q(u_h)) - I_{N,M}(Q(u_{h/2}))}{I_{N,M}(Q(u_{h/2}))}$$

which gives a total relative error of

$$\begin{aligned} &\frac{I_{N,M}(Q(u_h)) - E[Q(u)]}{E[Q(u)]} \\ &= \underbrace{\frac{E[Q(u_h)] - E[Q(u)]}{E[Q(u)]}}_{\text{bias error}} + \underbrace{\frac{I_{N,M}(Q(u_h)) - E[Q(u_h)]}{E[Q(u)]}}_{\text{statistical error}} \\ &\approx \frac{1}{1 - 1/2^p} \frac{I_{N,M}(Q(u_h)) - I_{N,M}(Q(u_{h/2}))}{I_{N,M}(Q(u_{h/2}))} + \frac{e_{N,M}(Q(u_h))}{I_{N,M}(Q(u_{h/2}))} \end{aligned} \quad \checkmark$$

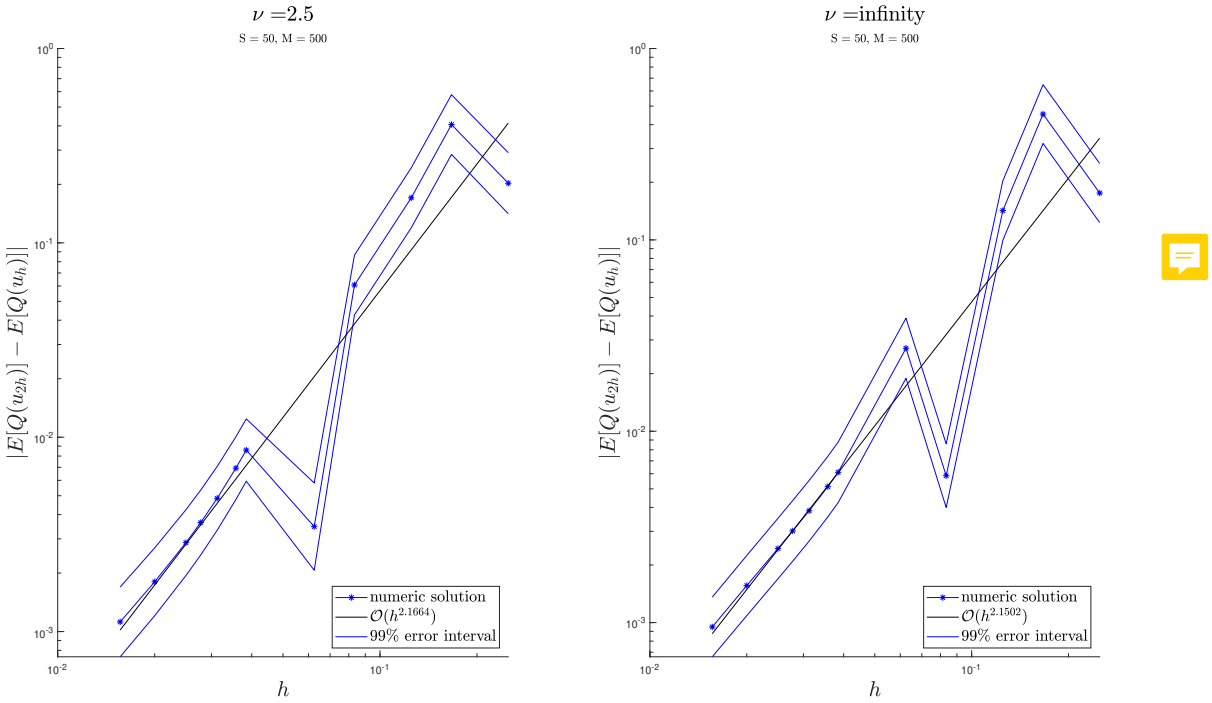

Figure 4: Estimating the order of convergence

For the order of convergence we choose values of $p = 2$ for both ν. To derive an estimate with a 0.1% tolerance we utilize an adaptive algorithm. We keep the number of shifts constant and adaptivly double the number of Sobol points M or half the stepsize h. The error split is given by

$$\text{Bias Error} \leq 0.5 \cdot TOL$$
$$\text{Statistical Error} \leq 0.5 \cdot TOL$$

	h	M	MC result	Stat Err	Bias Err
$\nu = 2.5$	0.125	1600	-1.6317	0.0318	0.0011
$\nu = \infty$	0.125	1600	-1.6562	0.0453	0.001

Table 1: Adaptive RQMC result

	h	M	MC result	Stat Err	Bias Err
$\nu = 2.5$	0.0625	5120	-1.5943	0.0367	0.0049
$\nu = \infty$	0.0625	5120	-1.6048	0.0396	0.0361

Table 2: Adaptive MC result

When comparing the result from Table (1) to the result of HW1 in Table (2) we see that the RQMC method has a comparable result and error, with a bigger stepsize and an about 3-times smaller samples size M. But in the RQMC method all M sobol sequences have been shifted $S = 50$ times

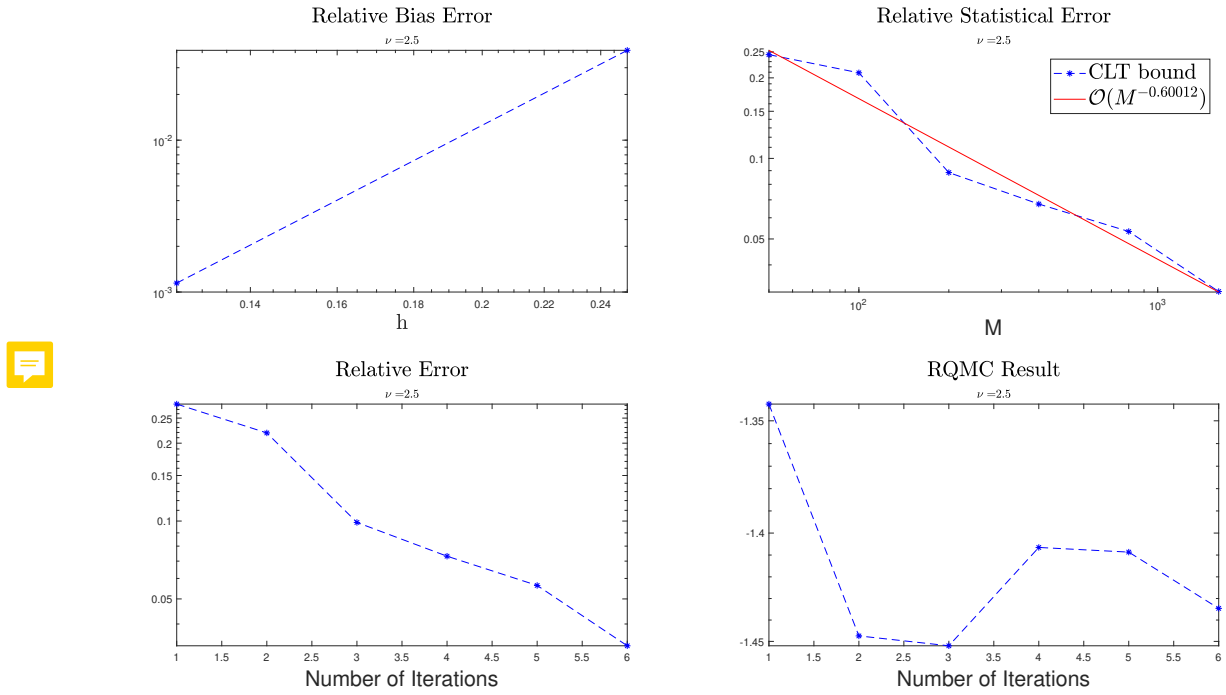

Figure 5: Adaptive RQMC result for $S = 50$ and $\nu = 2.5$

2.5.2

By denoting with C_1 the cost for one sample of $Q(u_{2h})$ and by C_2 the cost of one sample of $Q(u_h)$ we have a total cost of

$$C(M_1, M_2, S) = S(M_1 C_1 + M_2 C_2).$$

The Variance

$$Var = \frac{1}{S}\left(\frac{V_1}{M_1} + \frac{V_2}{M_2}\right)$$

where $V_1 = Var[Q(u_{2h})]$ and $V_2 = Var[Q(u_h)]$, because we take SM_1 and SM_2 samples respectively. We then get the Lagrangian

$$\mathcal{L} = S(M_1 C_1 + M_2 C_2) - \lambda\left(\left(\frac{TOL}{c_\alpha}\right)^2 - \frac{1}{S^2}\left(\frac{V_1}{M_1} + \frac{V_2}{M_2}\right)\right)$$

due to the constraint $\frac{c_\alpha\sqrt{Var}}{\sqrt{S}} \leq TOL$. From $\frac{\partial \mathcal{L}}{\partial M_1} = 0$ and $\frac{\partial \mathcal{L}}{\partial M_2} = 0$ we get

$$SC_l - \lambda\frac{V_l}{S^2 M_l^2} = 0, \quad l = 1, 2$$

$$\Rightarrow M_1 = \sqrt{\frac{\lambda V_1}{S^3 C_1}}, \quad M_2 = \sqrt{\frac{\lambda V_2}{S^3 C_2}}$$

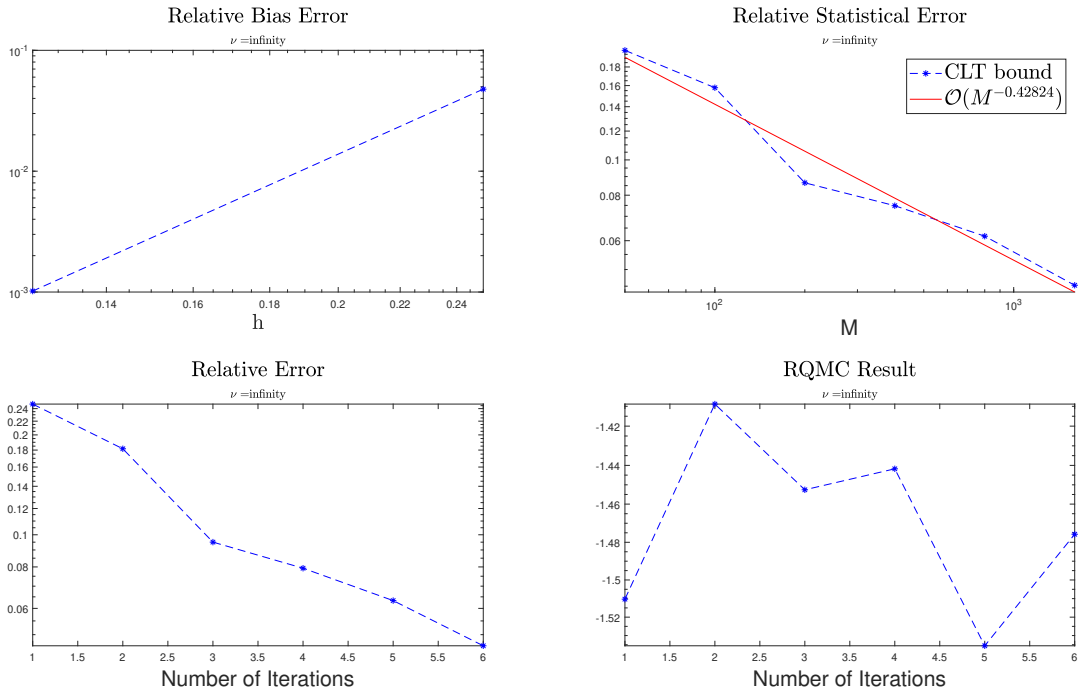

Figure 6: Adaptive RQMC result for $S = 50$ and $\nu = \infty$

Substituting this into the condition $\frac{\partial \mathcal{L}}{\partial \lambda} = 0$ gives

$$\begin{aligned} &\frac{1}{S^2}\left(\frac{V_1}{M_1} + \frac{V_2}{M_2}\right) - \left(\frac{TOL}{c_\alpha}\right)^2 = 0 \\ \Rightarrow &\frac{1}{S^2}\left(\frac{\sqrt{C_1 V_1 S^3}}{\sqrt{\lambda}} + \frac{\sqrt{C_2 V_2 S^3}}{\sqrt{\lambda}}\right) = \left(\frac{TOL}{c_\alpha}\right)^2 \\ \Leftrightarrow &\sqrt{\lambda} = \left(\frac{c_\alpha}{TOL}\right)^2 \left(\sqrt{\frac{C_1 V_1}{S}} + \sqrt{\frac{C_2 V_2}{S}}\right) \end{aligned}$$

To evaluate the CLT-bound for the RQMC bound we need $S \geq 2$. Because all the Sobol sequences are different we will shift each one just $S = 2$ times to reduce the computational cost. A higher S can decrease the statisical error and Variance, but we still see a reduced Variance compared to the results of Homework 1 in Table (4) at that of the Adaptive RQMC results in Table (5). Also compared to the Control Variate results from Homework 1 we see a reduced computational cost with a comparable approximation of the quantity of Interest.

	M1	M2	CV result	Variance	Computational Cost
$\nu = 2.5$	129	83	-1.5969	3.1601e+04	0.1188
$\nu = \infty$	118	84	-1.7256	2.4193e+04	0.1275

Table 3: Control Variate RQMC result

	M1	M	CV result	Variance	Computational Cost
$\nu = 2.5$	3490	903	-1.6428	9.3451e-04	0.6196
$\nu = \infty$	3855	1091	-1.5838	7.9600e-04	0.6534

Table 4: Control Variate MC result from Homework 1

	h	M	MC result	Variance	Computational Cost
$\nu = 2.5$	0.125	1600	-1.6317	0.0116	2.1287
$\nu = \infty$	0.125	1600	-1.6562	0.0248	1.9487

Table 5: Adaptive RQMC result

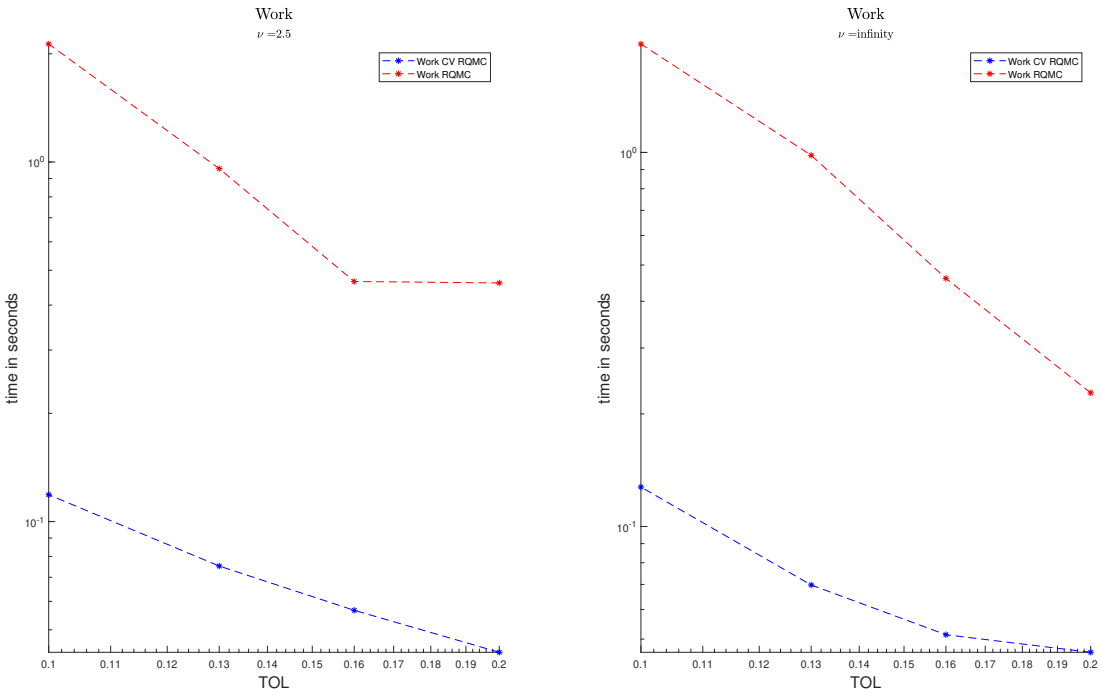

Figure 7: Work for the Control Variate and adaptive RQMC methods

The Costs C_1 and C_2 were estimated as an average over 100 realization. The Variances V_1 and V_2 were approximated with $M = 500$ and $S = 50$. The results are in figure (8) and (9).

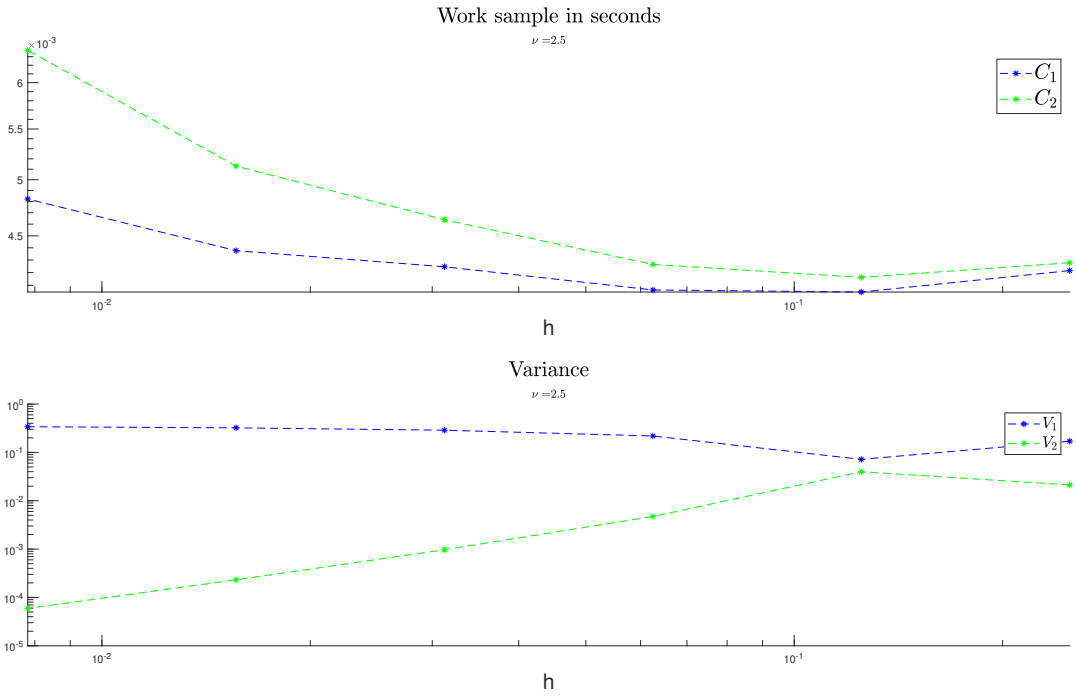

Figure 8: Cost and Variance estimates for $\nu = 2.5$

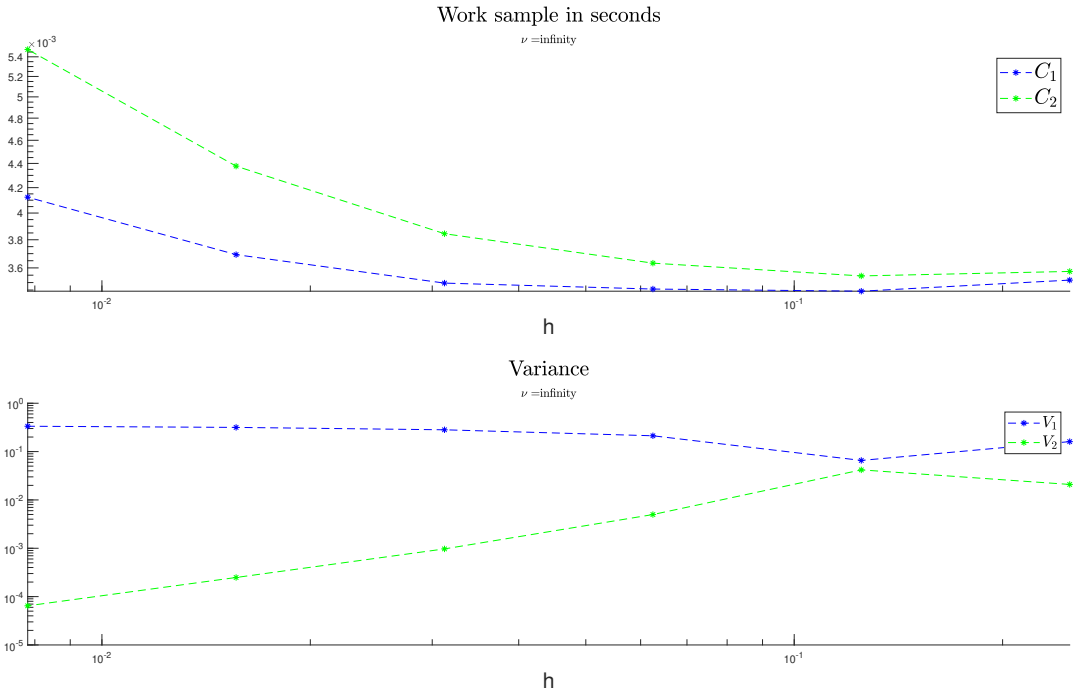

Figure 9: Cost and Variance estimates for $\nu = \infty$

2.5.3

Similar to Homework 1, in this task we are interested in the quantity $P(Q(u) < K)$ for different values $K \in \{-5, -10, -20\}$. We will first rewrite this quantity as an expected value

$$P(Q(u) < K) = \mathbb{E}[\mathbf{1}_{\{Q(u)<K\}}]$$

such that we can use RQMC to estimate this expectation. Again we will make use of Importance Sampling with a shift dilation technique to reduce variance. We estimate the statistical error using the Central limit theorem, the bias using the results from section 2.5.1 and adaptively choose the number of samples such that the total relative error gets below the tolerance level of 10%, i.e. TOL $= 0.1$. We used $I = 8$ number of grid points, as in question 1 (or $h = 0.125$, see table 1), and approximate u by u_h. Note that $u_h(\omega_m) = u_h(Y^{(m)})$, where $Y^{(m)}$ is a random variable with iid standart Gaussian. We will solve the same optimization problem as in Homework 1, namely

$$\mu^* = \text{argmax}_y \left\{ \mathbf{1}_{\{Q(u)<K\}} \prod_{n=1}^{N} \exp\left(-\frac{1}{2} y_n^2\right) \right\}.$$

Again, observe that this is an N-dimensional optimization problem. We can use the decaying nature of the Fourier coefficients, to reduce the dimensionality of this problem. As a cutoff-choice we choose $N = 5$ (same as in HW1) such that we get the same results as in homework 1 for the shifts. Now using the shifts from the optimization problem we can run the importance sampling technique in combination with RQMC to estimate the quantity such that the total relative error is below TOL $= 0.1$. In the table below you see results. Also figure 10 and figure 11 show the resulting CLT bounds of the RQMC procedure with and without Importance sampling, a plot of the corresponding RQMC estimate is also shown. We can see that the variance in comparison to Homework 1 is initially lower than the variance when using normal Monte Carlo instead of RQMC (with and without Importance Sampling). On the other hand, the number of samples needed to achieve increased drastically. This might be the case because of the mesh size which is significantly lower than the one used in HW1.

	K	M	$P(Q(u) < K)$	$\varepsilon_{\text{stat}}$	ε_{rel}
Model 2 $\nu = 0.5$	-5	1000	$1.83 \cdot 10^{-3}$	$8.94 \cdot 10^{-2}$	$9.69 \cdot 10^{-2}$
	-10	22500	$4.44 \cdot 10^{-5}$	$8.521 \cdot 10^{-2}$	$8.53 \cdot 10^{-2}$
	-20	$2 \cdot 10^5$	$5 \cdot 10^{-6}$	$9.78 \cdot 10^{-2}$	$9.81 \cdot 10^{-2}$
Model 2 $\nu = \infty$	-5	900	$4.4 \cdot 10^{-3}$	$7.98 \cdot 10^{-2}$	$8.14 \cdot 10^{-2}$
	-10	11000	$2.73 \cdot 10^{-4}$	$7.38 \cdot 10^{-2}$	$7.85 \cdot 10^{-2}$
	-20	$6 \cdot 10^5$	$6.67 \cdot 10^{-6}$	$9.116 \cdot 10^{-2}$	$9.12 \cdot 10^{-2}$

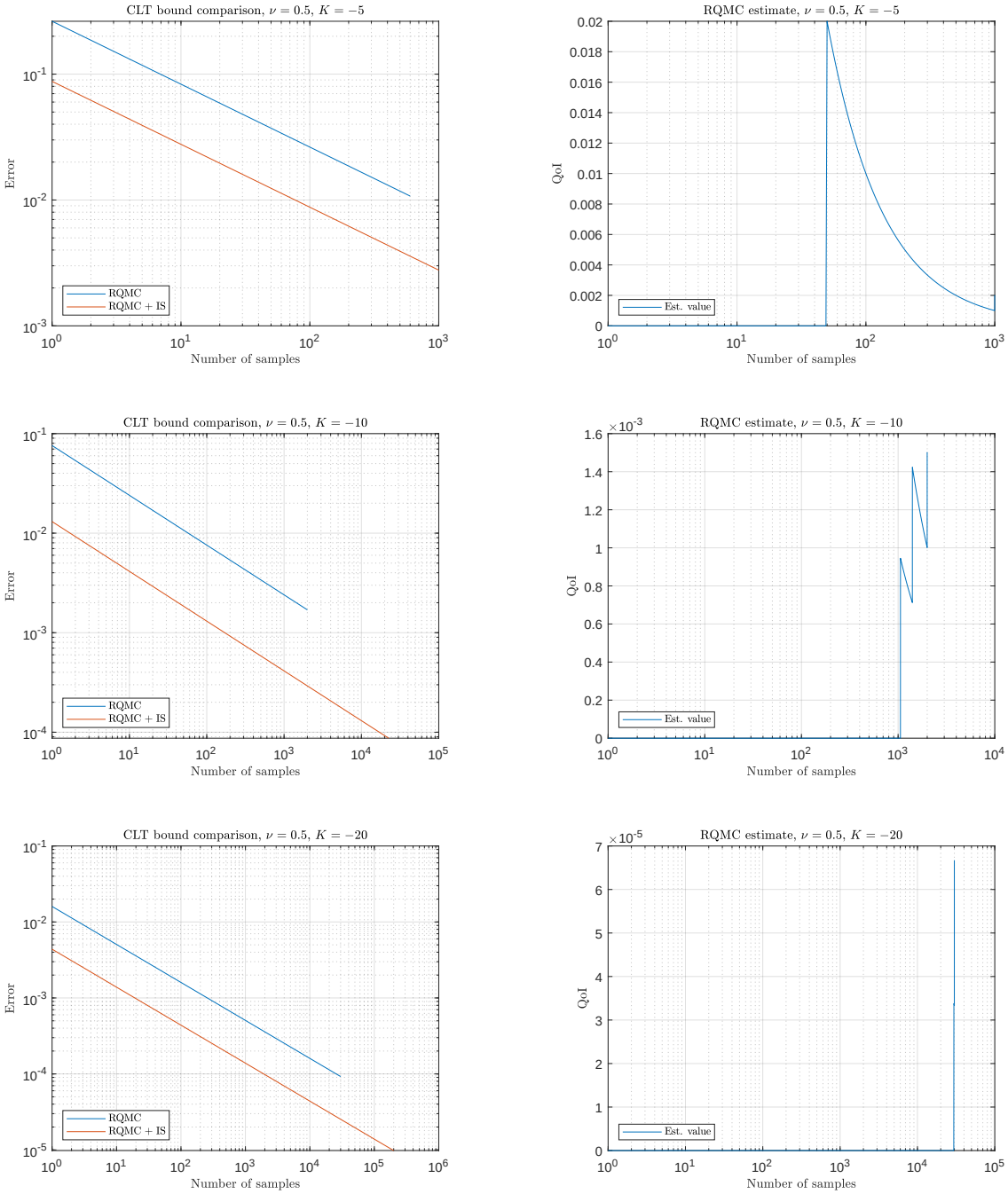

Figure 10: CLT bounds of RQMC with and without Importance sampling on the left, the RQMC estimate plotted against the number of samples on the right.

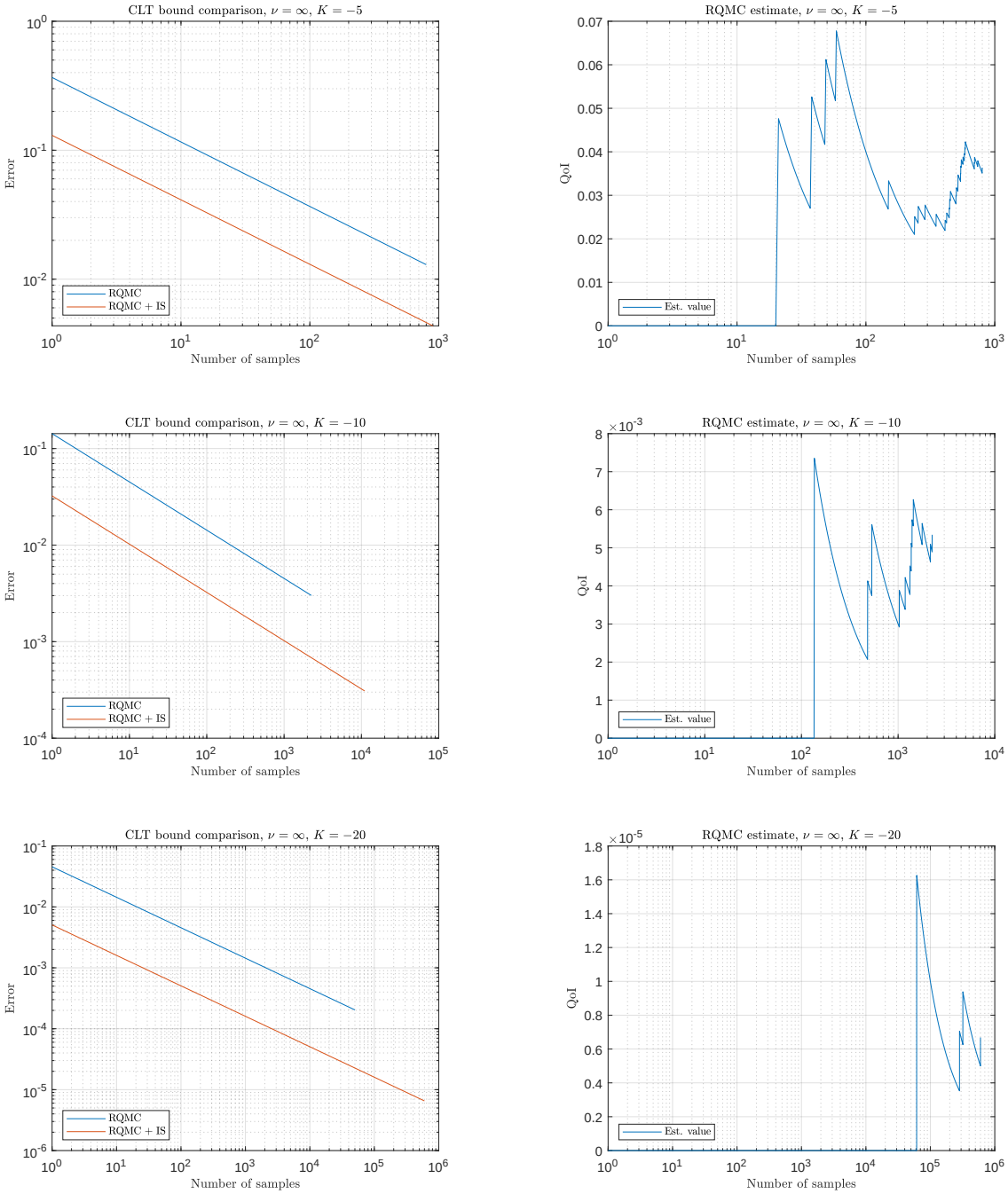

Figure 11: CLT bounds of RQMC with and without Importance sampling on the left, the RQMC estimate plotted against the number of samples on the right.

2.5.4

A comparison of the findings in this homework with homework 1 is included in the previous subtasks.

2.5.5

In this task we will propose two ways to estimate the same probabilities as in Task 2.5.3 using Large Deviation Theory (LDT).

(i) First we will use the following bound

$$|Q(u)| \leq \tilde{q}_0 \exp\left(\sum_{n\geq 1} \|b_n\|_\infty |Y_n|\right),$$

where $\tilde{q}_0$ and b_n, $n \geq 1$ are to be determined. Consider $D := (0,1)$ and the random elliptic PDE

$$-(a(x,\omega)u'(x,\omega))' = f(x), \quad \text{for } x \in D,$$

with $u(0,\cdot) = u(1,\cdot) = 0$ as stated in Task 2.2 (Problem). We are considering the linear bounded functional

$$Q(u) = \int_D u(x,\omega)\,\mathrm{dx}.$$

Now we know that the random field a can be approximated by the (random) expansion

$$\log(a) \approx b_0 + \sum_{n=1}^{N} b_n Y_n$$

where (b_n) are deterministic functions and (Y_n) are zero mean independent random variables, not necessarily identically distributed. Here we can use the Karhunen-Loeven expansion for the random field a, such that, following 2.4.2 from the Homework on possible approximations for the random field, we can write

$$a(x,\omega) = \exp(\kappa(x,\omega)) \approx \exp\left(\sum_{n=1}^{N} \sqrt{\lambda_n} e_n(x) Y_n(\omega)\right)$$
$$\iff \log(a(x,\omega)) \approx \sum_{n=1}^{N} b_n(x) \cdot Y_n(\omega)$$

where $b_n(x) := \sqrt{\lambda_n} \cdot e_n(x)$ and (λ_n, e_n) are the eigenvalues and corresponding eigenfunctions of the eigenvalue problem

$$\int_D C(x,y) e_n(y)\,\mathrm{dy} = \lambda_n e_n(x).$$

We know that (Y_n) are iid std. Gaussians and thus Y_n has bounded exponential moments. Now to estimate the probability $P(Q(u) < K)$ for some K we first estimate

$$|Q(u)| \leq \frac{\|Q\|_{H^{-1}(D)} C_D \|f\|_{L^2(D)}}{a_{\min}}$$

with the random variable

$$a_{\min}(\omega) = \min_{x \in D} a(x, \omega).$$

Now we use the hint and define the constant

$$\tilde{q}_0 := \frac{\|Q\|_{H^{-1}(D)} C_D \|f\|_{L^2(D)}}{\exp\left(\min_{x \in D} b_0(x)\right)}$$

such that we can further bound

$$|Q(u)| \leq \tilde{q}_0 \exp\left(\sum_{n=1}^{N} \|b_n\|_\infty |Y_n|\right)$$

yielding

$$P(Q(u) < K) \leq P\left(\exp\left(\sum_{n=1}^{N} \|b_n\|_\infty |Y_n|\right) < \frac{K}{\tilde{q}_0}\right). \quad \checkmark$$

To conclude, we use LDT estimates on

$$P(Q(u) < K) \leq P\left(\sum_{n=1}^{N} \|b_n\|_\infty |Y_n| < \log\left(\frac{K}{\tilde{q}_0}\right)\right). \quad \checkmark$$

To this end, introduce the centered random variables $\zeta_n = |Y_n| - \mathbb{E}[|Y_n|]$ and then $\checkmark$

$$P(Q(u) < K) \leq \exp\left(-I\left(\log\left(\frac{K}{\tilde{q}_0}\right) - \sum_{n=1}^{N} \|b_n\|_\infty \mathbb{E}[|Y_n|]\right)\right)$$

with

$$I(x) = \sup_\theta \left(\theta x - \sum_{n=1}^{N} \Lambda_{\zeta_n}(\theta \|b_n\|_\infty)\right). \quad \checkmark$$

The constant $\|Q\|_{H^{-1}(D)}$ can be determined exaclty. We have in general

$$\langle Q, v \rangle = \int_D Q^0 v + Q^1 v_x \, dx, \quad v \in H_0^1(D) \tag{1}$$

for functions $Q^0, Q^1 \in L^2(D)$. By definition

$$\langle Q, v \rangle = \int_0^1 v \, dx$$

and so $Q^1 = 1 \in L^2(0,1)$ and $Q^0 = 0 \in L^2(0,1)$ has to hold. We also have

$$\begin{aligned} \|Q\|_{H^{-1}(D)} &= \inf\left\{\left(\int_0^1 |Q^0|^2 + |Q^1|^2 \, dx\right)^{1/2} \,\middle|\, Q \text{ satisfies (1) for } Q^0, Q^1 \in L^2(0,1)\right\} \\ &= \left(\int_0^1 |1|^2 + |0|^2 \, dx\right)^{1/2} = 1 \end{aligned}$$

(ii) Now for the second way we use the Chernoff bound

$$P(Q(u) < K) \leq \exp(-I_{-Q(u)}(-K)),$$

where $I_{-Q(u)}(x) = \sup_{\theta>0}\{\theta x - \Lambda_{-Q(u)}(\theta)\}$ with

$$\Lambda_{-Q(u)}(\theta) = \log(\mathbb{E}[\exp(-\theta Q(u))].$$

Now for a given $h > 0$ and $\theta > 0$ we will approximate $\mathbb{E}[\exp(-\theta Q(u))]$ by

$$\mathbb{E}[\exp(-\theta Q(u))] \approx \frac{1}{M}\sum_{i=1}^{M} \exp(-\theta Q(u_h^{(i)})),$$

where $u_h^{(i)}$, $i = 1, \ldots, M$, are i.i.d. realizations of u_h. Then we use the same samples $u_h^{(i)}$, $i = 1, \ldots, M$, to approximate $I_{-Q(u)}(-K)$ numerically by repeating the same steps for several values of θ. For the range of θ we first chose $(0.1, 100)$ with a stepsize of 0.1. After that, realizing that the resulting θ are all in the range $(0, 1)$ we redid the optimization for θ on a finer grid on $(0, 1)$. As a choice of h and M we will choose the same as in Task 2.5.3 (adaptive importance sampling). The results can be seen in the table below.

	K	M	h	θ	$\exp(-I_{-Q(u)}(-K))$
Model 2 $\nu = 0.5$	-5	1000	0.125	0.4712	0.2921
	-10	22500	0.125	0.3054	0.1116
	-20	$2 \cdot 10^5$	0.125	0.2991	0.0084
Model 2 $\nu = \infty$	-5	900	0.125	0.1883	0.6515
	-10	11000	0.125	0.2459	0.1987
	-20	$6 \cdot 10^5$	0.125	0.1946	0.0492