STA 250 HOMEWORK 4
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Problem 1

In the first problem of this homework, I implemented the method proposed by Robert (2009) in CUDA code in order to obtain samples from a truncated normal distribution with given parameters. The distribution can be represented as

$$TN(\mu, \sigma^2; a, b)$$

where μ and σ^2 are the mean and variance of the original, i.e. untruncated, normal distribution and a, b represent the lower and upper bounds of the truncation interval with $a \geq -\infty, b \leq \infty$. Provided in the lecture notes, the expected values for a random variable $Z \sim TN(\mu, \sigma^2; a, b)$ is

$$E(Z) = \begin{cases} \mu - \sigma \frac{\phi(\frac{b-\mu}{\sigma})}{\Phi(\frac{b-\mu}{\sigma})} & \text{if } a = -\infty, b < \infty \\ \mu + \sigma \frac{\phi(\frac{a-\mu}{\sigma})}{1-\Phi(\frac{a-\mu}{\sigma})} & \text{if } a > -\infty, b = \infty \\ \mu + \sigma \frac{\phi(\frac{a-\mu}{\sigma}) - \phi(\frac{b-\mu}{\sigma})}{\Phi(\frac{b-\mu}{\sigma}) - \Phi(\frac{a-\mu}{\sigma})} & \text{if } a > -\infty, b < \infty \end{cases}$$

where ϕ, Φ are p.d.f and c.d.f of the standard normal distribution respectively. As directed in the paper by Robert (2009), when the truncation region is one-sided, for example $TN(0, 1; \mu^-, \infty)$, the algorithm for sampling from such truncated normal goes as follows:

(1) Generate a random sample $z = \mu^- + Expo(\alpha)$, where $Expo(\alpha)$ stands for a random number generated from the exponential distribution with parameter α.

(2) Compute the value $\psi(z)$ where

$$\psi(z) = \begin{cases} \exp(-\frac{(\alpha-z)^2}{2}) & \text{if } \mu^- < \alpha \\ \exp(-\frac{(\mu^- - \alpha)^2}{2}) \exp(\frac{(\alpha-z)^2}{2}) & \text{if } \mu^- \geq \alpha \end{cases}.$$

(3) Sample u from $U[0,1]$, if $u < \psi(z)$ then we accept z as our sample for this iteration; otherwise go back to step (1).

When the truncation region is one-sided but with an upper truncation, for example $TN(0,1;-\infty,\mu^+)$, we may simple reverse the sign of μ^+ and sample from lower truncation case then reverse the sign back. Also the optimal choice of parameter α for the exponential distribution is $\alpha_* = \frac{\mu^- + \sqrt{(\mu^-)^2+4}}{2}$.
When we have a two-sided truncation, e.g. $TN(0,1,;\mu^-,\mu^+)$, the algorithm is:

(1) Sample z from $U[\mu^-,\mu^+]$.

(2) Compute $\psi(z) = \begin{cases} \exp(-\frac{z^2}{2}) & \text{if } 0 \in [\mu^-,\mu^+] \\ \exp(-\frac{(\mu^-)^2-z^2}{2}) & \text{if } \mu^- > 0 \\ \exp(-\frac{(\mu^+)^2-z^2}{2}) & \text{if } \mu^+ < 0 \end{cases}$

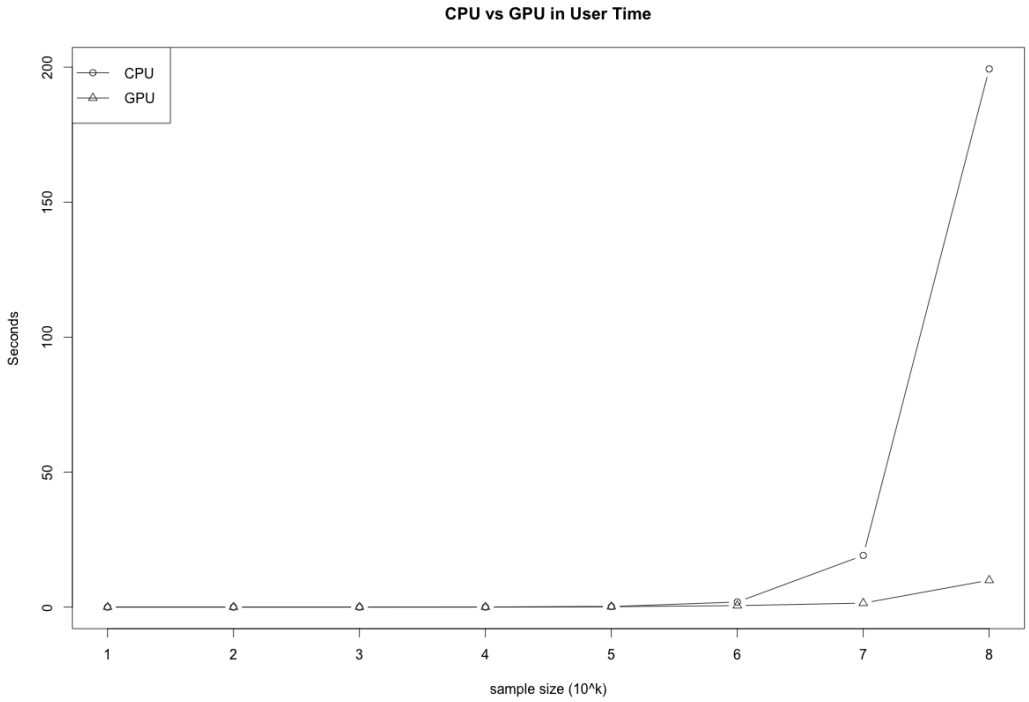
(3) Sample u from $U[0,1]$, if $u < \psi(z)$, we accept z; otherwise, go back to step (1).

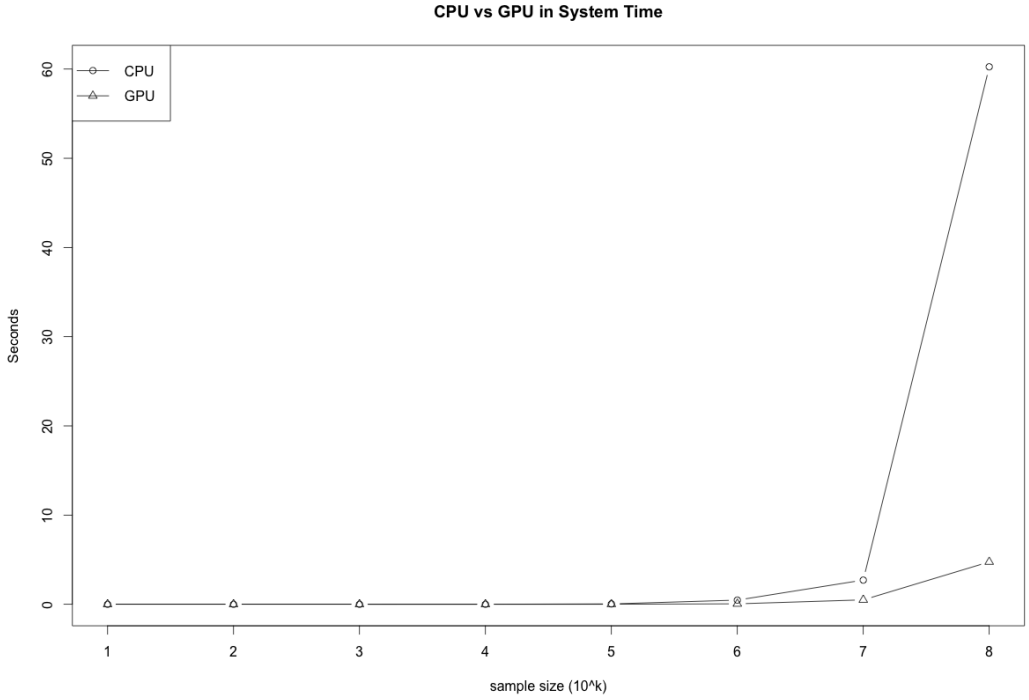
For any truncated normal distribution where $\mu \neq 0$ and/or $\sigma \neq 1$, we may simple use location-scale transformation to obtain properly transformed truncation region then transform the samples back to corresponding ones in the desired distribution.
After executing the code on AWS to generate 10000 samples from distribution $TN(2,1;0,1.5)$, the expected value was calculated to be 0.957, and the mean of samples were 0.849. The two values are not very close but not too far away. It could be due to some coding error when implementing the algorithm from Robert (2009).
Another trial was executed in R with the function rtnorm() from "msm" package to generate 10000 samples from the same truncated normal distribution. This time the mean of 10000 random samples turned out to be 0.954, which is quite close to the expected value.
Then both the CUDA and R code were put to test to generate 10^k samples, $k = 1, \cdots, 8$, still from the distribution $TN(2,1;0,1.5)$. The mean values for samples generated by GPU and CPU are

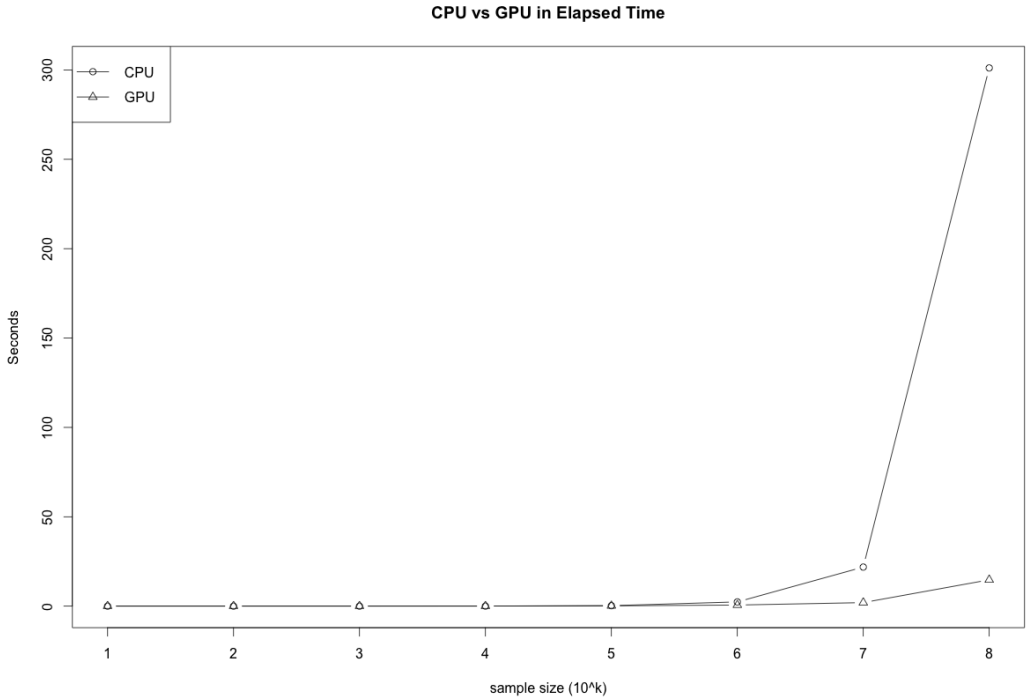
$k =$	1	2	3	4	5	6	7	8
GPU	0.871	0.812	0.843	0.849	0.849	0.849	0.849	0.849
CPU	1.343	0.946	0.950	0.954	0.957	0.957	0.957	0.957

Both CUDA and R codes returned "converged" mean values when sample size became large. However, the R code gave closer estimate of the expected value for the truncated normal distribution.

When looking at the cost/time of completing the tasks, GPU showed significant gain over CPU in terms of requiring less time to complete tasks when the sample size is large. The following are three figures, each for "User Time", "System Time" and "Elapsed Time":







Apparently when sample sizes are small ($k = 1, \cdots, 6$), GPU did not offer

much difference from CPU; however, when sample size got large ($k = 7, 8$), the time needed for CPU to complete each task grew exponentially, whereas GPU only required moderately more time than smaller sample sizes. Also most of the time increased for GPU was the "User Time", namely time needed transferring data between host and device.

For verification purposes, both CUDA and R codes were tested with three different truncated normal distributions: $TN(2, 1; -\infty, 0), TN(2, 1; 0, \infty)$, $TN(0, 1; -\infty, -10)$. 10000 samples were generated with GPU and CPU respectively, and the means are listed below together with expected values:

Distribution	$E(Z)$	GPU	CPU
$TN(2, 1; -\infty, 0)$	-0.373	-0.374	-0.374
$TN(2, 1; 0, \infty)$	2.055	2.057	2.057
$TN(0, 1; -\infty, -10)$	-10.098	-10.098	-10.098

The results in the table above showed that both my GPU and CPU code works for one-sided truncated normal distributions as well as in the tail region.

Problem 2

In this problem, we implemented Gibbs sampler algorithm for Probit MCMC, whose model is given by

$$\begin{aligned} Y_i|Z_i &\sim \mathbf{1}_{\{Z_i>0\}} \\ Z_i|\beta &\sim N(x_i^T\beta, 1) \\ \beta &\sim N(\beta_0, \Sigma_0) \end{aligned}$$

Firstly we need to set up the Gibbs sampler by finding marginal posterior distributions of $Z_i^{(t+1)}|Y_i, \beta^{(t)}$ and $\beta^{(t+1)}|Z_1^{(t+1)}, \cdots, Z_n^{(t+1)}$, i.e. in each iteration of Gibbs sampler, we want to sample Z_i's first, then update Z_i to sample β.

For $Z_i^{(t+1)}$ from the lecture note, we have

$$Z_i^{(t+1)}|Y_i, \beta^{(t)} \sim \begin{cases} TN(x_i^T\beta^{(t)}, 1; -\infty, 0) & \text{when } Y_i = 0 \\ TN(x_i^T\beta^{(t)}, 1; 0, \infty) & \text{when } Y_i = 1 \end{cases}$$

Next we need to obtain the marginal posterior distribution for $\beta^{(t+1)}|Z_1^{(t+1)}, \cdots, Z_n^{(t+1)}$. Let $X = (x_1^T, \cdots, x_n^T)^T, Z = (Z_1, \cdots, Z_n)^T$, then we can see that $Z|\beta \sim N(X\beta, \mathbf{I})$. So for the marginal posterior distribution of β, we have

$$\begin{aligned} p(\beta|Z) &\propto p(\beta)p(Z|\beta) \\ &\propto exp\{-\frac{1}{2}[(Z - X\beta)^T(Z - X\beta) + (\beta - \beta_0)^T\Sigma_0^{-1}(\beta - \beta_0)]\} \\ &\propto exp\{-\frac{1}{2}(\beta^T X^T X\beta - 2Z^T X\beta + \beta^T\Sigma_0^{-1}\beta - 2\beta_0^T\Sigma_0^{-1}\beta)\} \end{aligned}$$

By Bayesian theory, given the facts that β has a normal prior distribution and the distribution of $Z|\beta$ is also normal, the posterior distribution for β should also be normal, more precisely multivariate normal distribution. We can extract the parameters of that normal distribution from the above quadratic expression of β:

$$\begin{aligned} &\beta^T X^T X\beta - 2Z^T X\beta + \beta^T\Sigma_0^{-1}\beta - 2\beta_0^T\Sigma_0^{-1}\beta \\ &= \beta^T(X^T X + \Sigma_0^{-1})\beta - 2(Z^T X + \beta_0^T\Sigma_0^{-1})\beta \end{aligned}$$

If $\beta \sim N(\mu_\beta, \Sigma_\beta)$, then the quadratic expression would contain the following terms:

$$\beta^T\Sigma_\beta^{-1}\beta - 2\mu_\beta^T\Sigma_\beta^{-1}\beta$$

Matching corresponding terms in the expression, we get

$$\begin{aligned}
\Sigma_\beta^{-1} &= (X^T X + \Sigma_0^{-1}) \\
\Rightarrow \Sigma_\beta &= (X^T X + \Sigma_0^{-1})^{-1} \\
\mu_\beta^T \Sigma_\beta^{-1} &= (Z^T X + \beta_0^T \Sigma_0^{-1}) \\
\Rightarrow \Sigma_\beta^{-1} \mu_\beta &= (Z^T X + \beta_0^T \Sigma_0^{-1})^T \\
&= (\Sigma_0^{-1} \beta_0 + X^T Z) \\
\Rightarrow \mu_\beta &= \Sigma_\beta \Sigma_\beta^{-1} \mu_\beta \\
&= (X^T X + \Sigma_0^{-1})^{-1} (\Sigma_0^{-1} \beta_0 + X^T Z)
\end{aligned}$$

Therefore we obtain the second step in Gibbs sampler: sample $\beta^{(t+1)}|Z^{(t+1)}$ from multivariate normal distribution

$$N[(X^T X + \Sigma_0^{-1})^{-1}(\Sigma_0^{-1}\beta_0 + X^T Z^{(t+1)}), (X^T X + \Sigma_0^{-1})^{-1}]$$

Overall the Gibbs sampler generally goes:

(1) Initialize by setting β_0, Σ_0 and $t = 0$.

(2) Obtain the vector $Z^{(t+1)}$ by sampling each $Z_i^{(t+1)}$ from corresponding truncated normal distribution, either $TN(x_i^T \beta^{(t)}, 1; -\infty, 0)$ when $Y_i = 0$ or $TN(x_i^T \beta^{(t)}, 1; 0, \infty)$ when $Y_i = 1$.

(3) Sample $\beta^{(t+1)}$ from the multivariate normal distribution given above.

(4) Check for convergence, if not, increment t to $t + 1$, go to step (2) and iterate.

In our case, we set $\beta_0 = \mathbf{0}, \Sigma_0 = \mathbf{I}$. Since the homework mainly focused on comparing CPU and GPU performances, the convergence of generated Markov chain was not tested. For the CPU code, I programmed the algorithm in R. For the GPU code, the only part completed on GPU was sampling $Z^{(t+1)}$ by using .cuda() to call the kernel function coded in problem 1, and the rest goes very similarly to CPU code in R. With provided R script, five datasets was simulated; however only the first four datasets were used, because the

last one was quite large and not feasible to compute within reasonable time. Additionally only 600 iterations were executed for each dataset with the first 100 deemed as "burnin" iterations. After verifying that both CPU and GPU codes worked with the mini dataset, they were executed on the first four datasets as described before. It did not take long for GPU code to finish the Probit MCMC with all four datasets, while the CPU code took a much longer time to finish, especially when the size of dataset gets large. The results are displayed as following (elapsed time in seconds):

Dataset	size n	Time for GPU	Time for CPU
1	1000	22.801	205.796
2	10000	24.145	2155.732
3	100000	40.034	15442.380
4	1000000	190.982	NA

Perhaps the CPU code I programmed was not very efficient but it was still obvious that GPU offered huge savings in computation time especially as the size of dataset gets large. Note that the fourth dataset took extremely long time and had to be forcefully terminated without returning any result.
It is apparent that in this problem, GPU gave a huge performance boost when carrying out Probit MCMC, particularly sampling from a truncated normal distribution. Even if the efficiency of CPU code got improved, judging by the result, GPU would remain to perform better especially when we have a dataset with large number of observations. For instance, when n increased from 10000 to 100000, GPU code only took less than twice as much time as needed for smaller n, whereas CPU code took more than seven times. The results showed that GPU/CUDA gives a lot of advantages in speed when the size of dataset increases and task is reasonably simple to handle by threads on the device.

Discussion for Both Problems

The focus of this homework was to learn to program in CUDA and carry out certain tasks on GPUs. When writing CUDA code in the .cu file, I did not follow the skeleton exactly and only used the algorithms proposed by Robert

(2009) without trying rejection sampling first. Given the efficiency of C, the code performed relatively well, with most tasks finished in a matter of seconds to several minutes, compared to CPU code in R which took many minutes or even hours. Furthermore, the "recycling" was not handled in CUDA code, since such operation can be executed in R quickly; hence arguments "mu" and "sigma" were always vectors of length N when passed to the kernel function. It was noticeable that when the truncation was one-sided, my CUDA code returned very close results to CPU code and theoretical values. But in the two-sided truncation case, GPU did not return a quite close result; it could either be due to the algorithm itself or some flaw in my code, which was not detected when I checked my code against the algorithm in the reference paper.