ESAM 448 Random Processes Homework 2

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Problem 1: Monte-Carlo Integration

Use Monte-Carlo integration to evaluate the integrals below. Use M sample points X_j and determine the Monte-Carlo estimate $\hat{I}$ of the integral as well as an estimate for the standard error of the mean $\hat{\sigma}_I$. To understand the accuracy of the integration obtain $N = 500$ estimates of $\hat{I}$ and of $\hat{\sigma}_I$. Then plot the mean across N_{trial} of the absolute value of the error, i.e.,

$$E_m = \frac{1}{N_{trial}} \sum_{j_{trial}} |\hat{I}_{j_{trial}} - I_{exact}|,$$

as well as the corresponding standard deviation $\mathrm{std}(\hat{I})$ and the average $\langle \hat{\sigma}_I \rangle$ of $\hat{\sigma}_I$ acorss the N_{trials} as a function of $M = 4^p$, with p up to $p = 9$. Use `loglog` for these plots. Why?

(a)

$$\int_0^\infty \cos x e^{-x} \, \mathrm{d}x$$

How do the three quantities $\langle \hat{I} \rangle$, $\langle \hat{\sigma}_I \rangle$ and $\mathrm{std}(\hat{I})$ scale with M? Why?

(b) Now consider the integral

$$\int_0^\infty x^{-\alpha} e^{-x} \, \mathrm{d}x,$$

using $g(x) = x^{-\alpha}$ and $p(x) = e^{-x}$. Perform the above analysis for $\alpha = \frac{1}{4}$ and for $\alpha = \frac{3}{4}$. Discuss the difference in the outcome of the two cases. To get insight into your results consider the analytical expression for $\mathrm{Var}[g(x)]$ for general α. Is $\mathrm{Var}[g(x)]$ finite for all α?

(c) Now use Monte-Carlo integration for the integral

$$\int_0^{x_{max}} x^{-\alpha} e^{-x} \, \mathrm{d}x, \quad \text{with } \alpha = \frac{3}{4} \text{ and } x_{max} = 2,$$

but use $g(x) = e^{-x}$ and $p(x) = e^{-\alpha}$. Discuss the outcome in view of your results of part 1b.

(d) Based on your results in parts 1b and 1c, what approach would you use to compute the integral in part 1b reliable for $\alpha = \frac{3}{4}$.

(a) Let $g(x) = \cos x$ and $p(x) = e^{-x}$. We compute the Monte-Carlo approximation $\hat{I}$ N times using

$$\hat{I} = \frac{1}{M}\sum_{i=1}^{M} g(X_i),$$

where X_i are random numbers drawn from distribution $p(x)$. After each Monte-Carlo approximation, we compute the estimate of the standard error of the mean

$$\hat{\sigma}_{\hat{I}} = \left(\frac{1}{M}\frac{1}{M-1}\sum_{i=1}^{M}(g(X_i) - \hat{I})^2\right)^{\frac{1}{2}}.$$

In Figure 1, we plot the Monte-Carlo approximation $\hat{I}$ against p and plot $\log(E_m)$, $\log(\langle\hat{\sigma}_I\rangle)$, and $\log(\mathrm{std}(\hat{I}))$ against log(M). The slopes of the three `loglog` plots are 0.5, meaning E_m,($\langle\hat{\sigma}_I\rangle$), and $\mathrm{std}(\hat{I})$ scale like $M^{-1/2}$. So we need to quadruple M in order to decrease the approximation error by half.

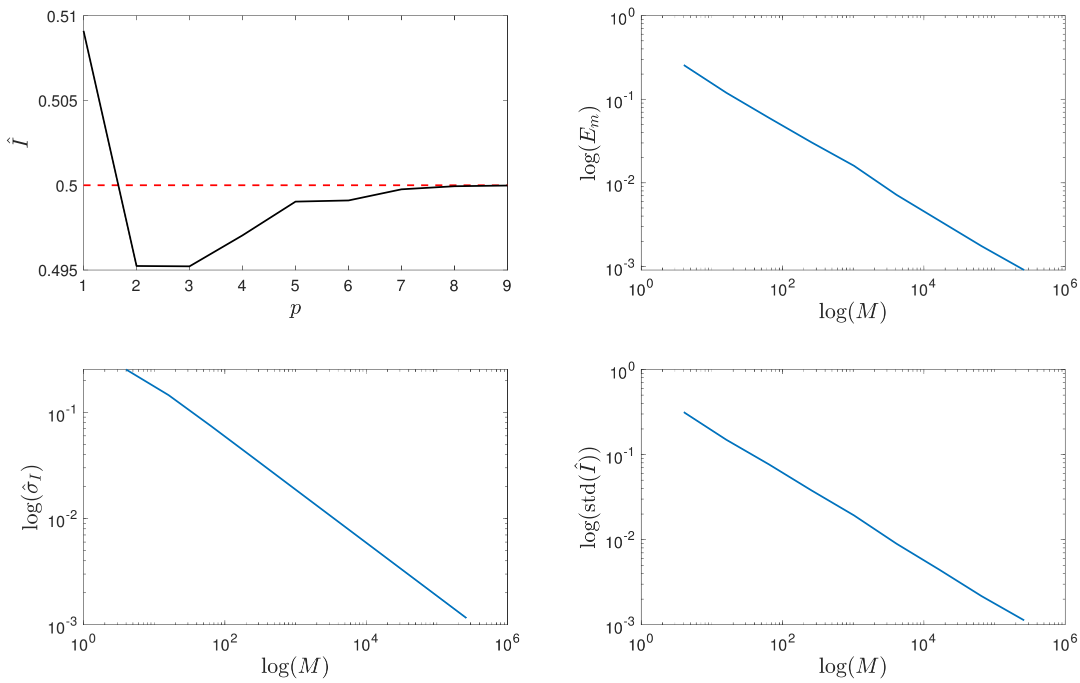


Figure 1: Monte-Carlo approximation of $\int_0^\infty \cos x e^{-x}\,\mathrm{d}x$

(b) To evaluate the integral

$$\int_0^\infty x^{-\alpha} e^{-x} \, \mathrm{d}x,$$

we let $g(x) = x^{-\alpha}$ and $p(x) = e^{-x}$ and repeat the procedures in (a). The same plots are produced in Figures 2 and 3, for $\alpha = 1/4$ and $3/4$, respectively.

The Monte-Carlo approximation for $\alpha = 1/4$ appears accurate and the errors scale like $M^{-1/2}$. For $\alpha = 3/4$, the approximation has lower accuracy and `loglog` plots for the error terms are not straight lines when the number of sampling points is less than 10^4. By the central limit theorem, the number of sampling points needed to achieve certain accuracy grows with the variance of $g(x)$, i.e.,

$$N \propto \frac{\text{Var[g(x)]}}{\Delta\mu^2},$$

where $\Delta\mu$ is the error for a given confidence level. To assess the accuracy of our approximation, we calculate the variance of $g(x) = x^{-\alpha}$:

$$\begin{aligned} \mathrm{Var}[g(x)] =& \mathrm{E}[g(x)^2] - \mathrm{E}[g(x)]^2 \\ =& \int_0^\infty g(x)^2 p(x) \, \mathrm{d}x - \left(\int_0^\infty g(x)p(x) \, \mathrm{d}x \right)^2 \\ =& \int_0^\infty x^{-2\alpha} e^{-x} \, \mathrm{d}x - \left(\int_0^\infty x^{-\alpha} e^{-x} \, \mathrm{d}x \right)^2 \\ =& \Gamma(1-2\alpha) - \Gamma(1-\alpha)^2. \end{aligned}$$

Note that $\mathrm{Var}[g(x)]$ is singular when $\alpha = n/2, n = 1, 2, \cdots$, and

$$\begin{aligned} \mathrm{Var}[g(x)] &= \sqrt{\pi} - \Gamma(3/4) \approx 0.27 \quad \text{for } \alpha = 1/4; \\ \mathrm{Var}[g(x)] &= -2\sqrt{\pi} - \Gamma(1/4) \approx -16.69 \quad \text{for } \alpha = 3/4. \end{aligned}$$

Since $\mathrm{Var}(x^{-3/4}) \ll \mathrm{Var}(x^{-}1/4)$, with the same amount of sampling points M, the Monte-Carlo approximation for $\alpha = 3/4$ is worse than the approximation for $\alpha = 1/4$.

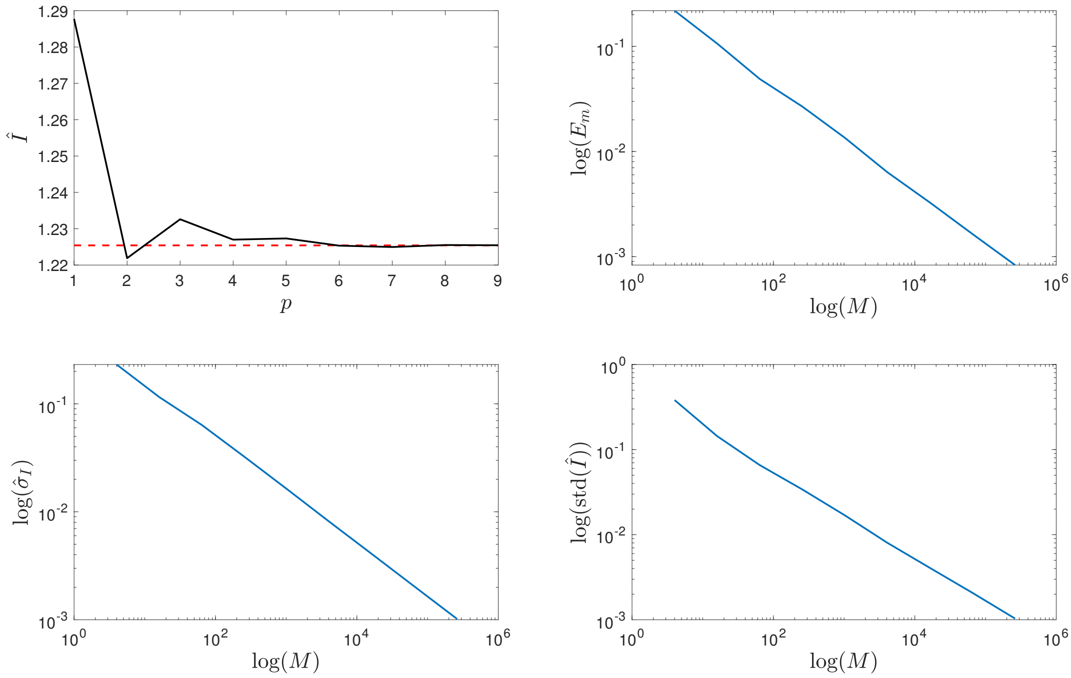


Figure 2: Monte-Carlo approximation of $\int_0^\infty x^{-\alpha}e^{-x}\,\mathrm{d}x$ with $\alpha = 3/4$.

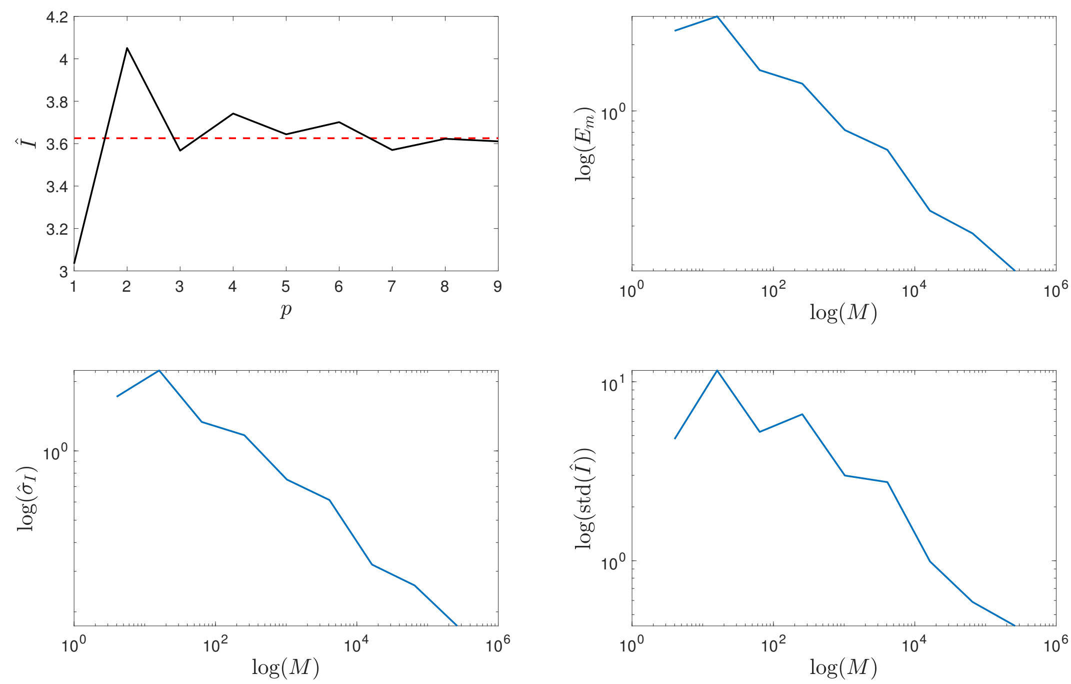


Figure 3: Monte-Carlo approximation of $\int_0^\infty x^{-\alpha}e^{-x}\,\mathrm{d}x$ with $\alpha = 3/4$.

(c) Now we consider the integral

$$\int_0^2 x^{-3/4} e^{-x} \, \mathrm{d}x.$$

We evaluate the integral using Monte-Carlo method with $g(x) = e^{-x}$ and $p(x) = x^{-3/4}$. As shown in Figure 4, the approximation has $O(M^{-1/2})$ convergence (the slopes of the `loglog` plots are 0.5).

Note that the integrals in (b) and (c) have the same integrands but very different approximation results. This is because when we use $g(x) = e^{-x}$, the variance of $g(x)$ is greatly reduced and thus fewer sampling points are needed to achieve the same accuracy:

$$\begin{aligned}
\mathrm{Var}[g(x)] =& \mathrm{E}[g(x)^2] - \mathrm{E}[g(x)]^2 \\
=& \int_0^\infty g(x)^2 p(x) \, \mathrm{d}x - \left(\int_0^\infty g(x) p(x) \, \mathrm{d}x \right)^2 \\
=& \int_0^2 \left(4\sqrt[4]{2} e^{-x} \right)^2 \left(\frac{x^{-3/4}}{4\sqrt[4]{2}} \right) \, \mathrm{d}x - \left(\int_0^2 \left(4\sqrt[4]{2} e^{-x} \right) \left(\frac{x^{-3/4}}{4\sqrt[4]{2}} \right) \, \mathrm{d}x \right)^2 \\
\approx& 1.8.
\end{aligned}$$

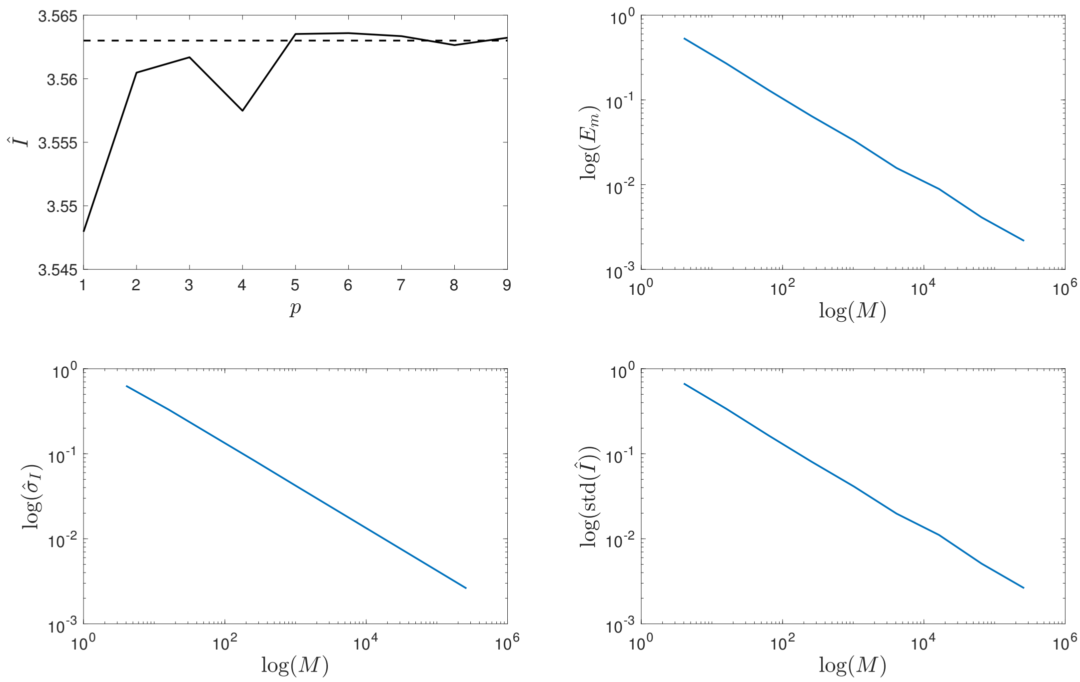


Figure 4: Monte-Carlo approximation of $\int_0^2 x^{-\alpha}e^{-x}\ \mathrm{d}x$ with $\alpha = 1/4$.

(d) Based on the results in (b) and (c), I would use $p(x) = x^{-3/4}$ and $g(x) = e^{-x}$ to evaluate the integral in (b) so that the situation with large $\mathrm{Var}[g(x)]$ can be avoided and we would need fewer sampling points to achieve good accuracy.

Problem 2: Phase Transition in the Ising Model

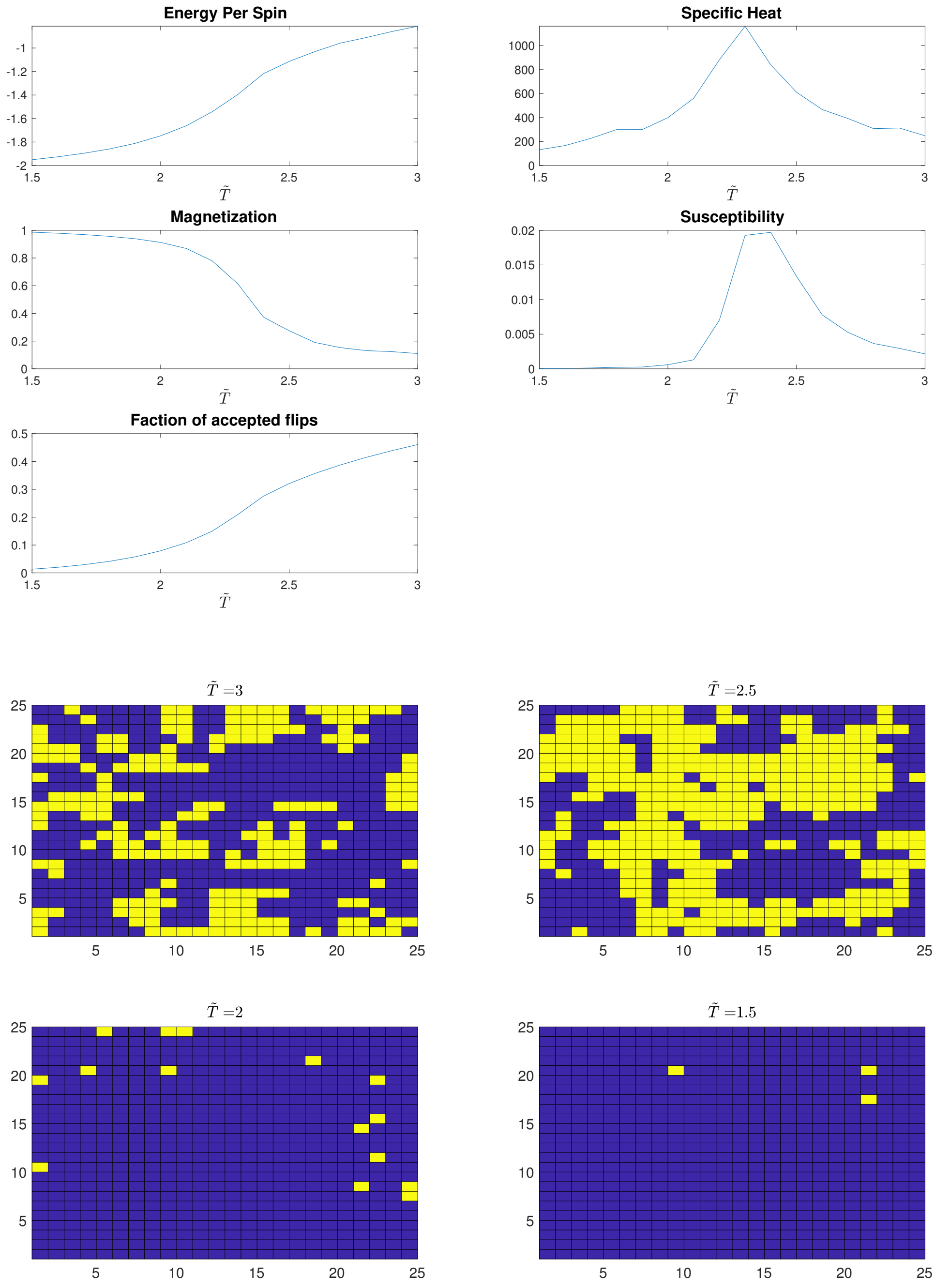
Implement the metropolis algorithm for the Ising model on a square lattice of size $L \times L$ with periodic boundary conditions.

(a) For $H = 0, J = 1, L = 25, t_{corr} = 200, N_{trial} = 400$, plot graphs of the following quantities vs. temperature in the range $\tilde{T} \in [1.5, 3]$ in steps of $\Delta\tilde{T} = 0.1$:

1. Energy per pin: $\langle U(\tilde{T})\rangle = \frac{1}{L^2}\sum_{\vec{\sigma}} U(\vec{\sigma})p(\vec{\sigma}, \tilde{T})$;
2. Specific Heat: $\frac{1}{\tilde{T}^2}\left(\langle U(\tilde{T})^2\rangle - \langle U(\tilde{T})\rangle^2\right)$;
3. Magnetization per pin: $m(\tilde{T}) = \langle |M(\vec{\sigma})|\rangle = \sum_{\vec{\sigma}} |M(\vec{\sigma})|p(\vec{\sigma}, \tilde{T})$, where $M(\vec{\sigma}) = \frac{1}{L^2}\sum_{i,j}\sigma_{i,j}$;
4. Susceptibility: $\frac{1}{\tilde{T}}\left(\langle M(\vec{\sigma})^2\rangle - \langle |M(\vec{\sigma})|\rangle^2\right)$
5. Fraction of accepted spin flips
6. For 3 representative values of the temperature plot a snapshot of the final spin configuration $\vec{\sigma}$ and comment on them.

(b) L. Onsager showed analytically that in the thermodynamic limit $L \to \infty$ this model has a phase transition at a temperature $\tilde{T}_c$ such that $\tilde{T} > \tilde{T}_c$ the magnetization vanishes, $m(\tilde{T}) = 0$, while when $\tilde{T}$ is decreased below $\tilde{T}_c$ the magnetization increases continuously. Moreover, the susceptibility diverges at $\tilde{T}_c$. Do your computations for $L = 25$ show behavior resembling these theoretical results? change your parameter in a way that provides a more convincing confirmation of the theory.

(a) In Figure 5, we observe that as $\tilde{T}$ decreases, the magnetization per pin increases and the energy per spin decreases. Both specific heat and the susceptibility peak between $\tilde{T} = 2$ and $\tilde{T} = 2.5$. The fraction of accepted flips also decreases as $\tilde{T}$ becomes lower. In the snapshots of final spin configurations, fewer spin flips occur when $\tilde{T}$ is low ($\tilde{T} \leq 2$) and the configurations appear uniform.



Energy Per Spin
Specific Heat
Magnetization
Susceptibility
Faction of accepted flips
$\tilde{T}$
$\tilde{T}$ =3
$\tilde{T}$ =2.5
$\tilde{T}$ =2
$\tilde{T}$ =1.5

Figure 5: $L = 25$

(b) See Figure 6:

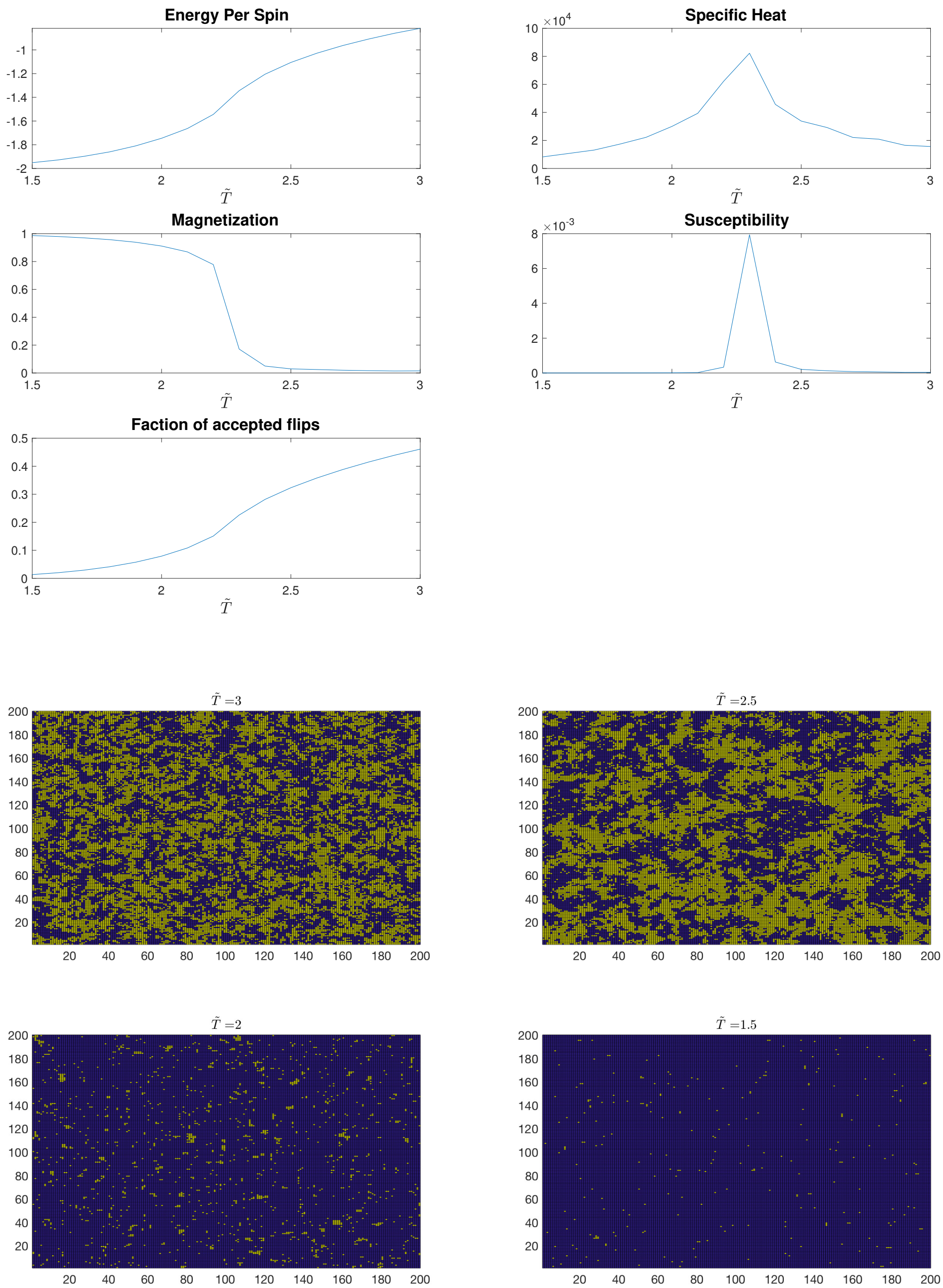


Figure 6: $L = 200$

To confirm L.Onsager's theory as L limits to infinity, we take $L = 200$ and repeat the algorithm (other parameters are fixed). In Figure 6, we observe that the magnetization per spin becomes very close to zero for $\tilde{T} > 2.4$, and for $\tilde{T} < 2.4$, the magnetization per spin increases as $\tilde{T}$ increases. If we assume $\tilde{T}_c$ is near $\tilde{T} = 2.4$, then our numerical results are consistent with the analytic results in Onsager's paper.

Also, we find that the susceptibility of the system remain low for all $\tilde{T}$ except for near $\tilde{T}_c = 2.4$, where there is a sharp peak. This agrees with Onsager's theory that the susceptibility diverges at $\tilde{T}_c$.