XY

Practical Numerical Simulations
Assignment 3

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1 The XY Model

The XY model is an O(2) model for simulating statistical mechanics on a 2-dimensional lattice Λ. Specifically, it is useful for simulating spin-statistics. It is the special case of $n = 2$ in the n-vector model and is thus analogous to the Ising ($n = 1$) and Heisenberg ($n = 3$) models.

In comparison to the more familiar Ising model whose spins take discrete values, i.e. $\sigma_x \in (\uparrow, \downarrow)$, the spins of the XY model take on continuous values, $\sigma_{\mathbf{x}} \in \mathrm{U}(1)$. Here $\mathbf{x} = (x_1, x_2) \in \Lambda \subset \mathbb{Z}^2$ is the lattice site on which the spin takes values. We can therefore represent the spins as $\sigma_{\mathbf{x}} = \exp(i\theta_{\mathbf{x}})$ with $\theta_{\mathbf{x}} \in (-\pi, \pi]$.

The action of the XY model is given by

$$\begin{aligned} S(\theta) &= \sum_{\mathbf{x},\mathbf{y}\in\Lambda} 1 - \Re(\sigma_{\mathbf{x}}{}^{*}\sigma_{\mathbf{y}}) \\ &= \sum_{\mathbf{x},\mathbf{y}\in\Lambda} 1 - \cos(\theta_{\mathbf{x}} - \theta_{\mathbf{y}}). \end{aligned} \tag{1.1}$$

Assuming only nearest neighbour interactions,

$$\mathbf{y} \in n(\mathbf{x}) = \{(x_1+1, x_2), (x_1-1, x_2), (x_1, x_2+1), (x_1, x_2-1)\},$$

the set of nearest neighbours to $\mathbf{x}$.

$$\begin{array}{ccc} & \sigma_{(x_1,x_2+1)} & \\ \sigma_{(x_1-1,x_2)} & \sigma_{(x_1,x_2)} & \sigma_{(x_1+1,x_2)} \\ & \sigma_{(x_1,x_2-1)} & \end{array}$$

2 The Count of Monte Carlo

The law of large numbers implies that expectation values may be calculated by sampling the value and computing the sample mean. Thus, we may in principle use Monte Carlo methods to evaluate expectation values of stochastic variables.

The lattice* is initialised with a "hot start", i.e. the spins are brought into life in a disordered phase. We must generate new states from this via a Markov process.

The Metropolis algorithm is used to generate a Markov chain of spin configurations. This procedure reversibly creates a new spin at a lattice site, computes the action for the new spin configuration, S', and compares the two actions S, S'. The comparison is made using the fixed-point sampling probability density

$$\pi(S) = \frac{1}{Z}\exp(-\beta S)$$

*The lattice Λ is topologically a torus, as each dimension has been compactified cyclically.

where Z is the partition function given in equation 3.2 and $\beta = \frac{1}{k_B T}$ is the Boltzmann factor. The ratio

$$\begin{aligned}\frac{\pi(S')}{\pi(S)} &= \frac{e^{-\beta S'}}{e^{-\beta S}} \\ &= e^{\beta(S-S')} = r,\end{aligned}$$

so if $r > 1$, we accept the new spin configuration as it has minimised the action. If $r < 1$, we accept the new configuration with a certain probability, determined by `drand48()`, else it is rejected.

A function then runs Metropolis over all lattice sites and updates the lattice accordingly. This is done in a checkerboard fashion, running over first the even and then odd sites.

In this manner, for a given β and a large enough number of iterations, the system will reach a stable state. This state will be one of either order or disorder, determined by β. The mysterious transition between these states is the topic of §3.

3 The Kosterlitz–Thouless Transition

The Mermin–Wagner theorem states that in dimension $d \leq 2$, spontaneous symmetry breaking at finite energy cannot occur in systems with short-range interactions. This admits a new class of phase transitions, topological phase transitions, which allow for distinct stable states.

The transition is called "topological" because the existence of the high temperature stable state is dependent on topological defects in the configuration. These topological defects are manifest as vortices, whose existence becomes thermodynamically favourable above the transition energy. Thus, the phases before and after the transition are different topological spaces in the homotopic sense and the transition brings these different topologies about.

The Kosterlitz–Thouless transition is an infinite order topological phase transition. In the Ehrenfest classification, this means there does not exist a finite n such that

$$\left(\frac{\partial^n g_1}{\partial T^n}\right) \neq \left(\frac{\partial^n g_2}{\partial T^n}\right), \qquad \left(\frac{\partial^n g_1}{\partial P^n}\right) \neq \left(\frac{\partial^n g_2}{\partial P^n}\right)$$

for g_1, g_2 the specific Gibbs free energy of the distinct phases. In a more modern sense, this means the transition is continuous and breaks no symmetries.

By Hamilton's principle, the variation of the action δS gives the equations of motion. Note that when $\theta_{\mathbf{x}} \approx \theta_{\mathbf{y}}$, $\cos(\theta_{\mathbf{x}} - \theta_{\mathbf{y}}) \approx 1$. Therefore in the limit,

$$\lim_{\theta_{\mathbf{x}} \to \theta_{\mathbf{y}}} S = 0.$$

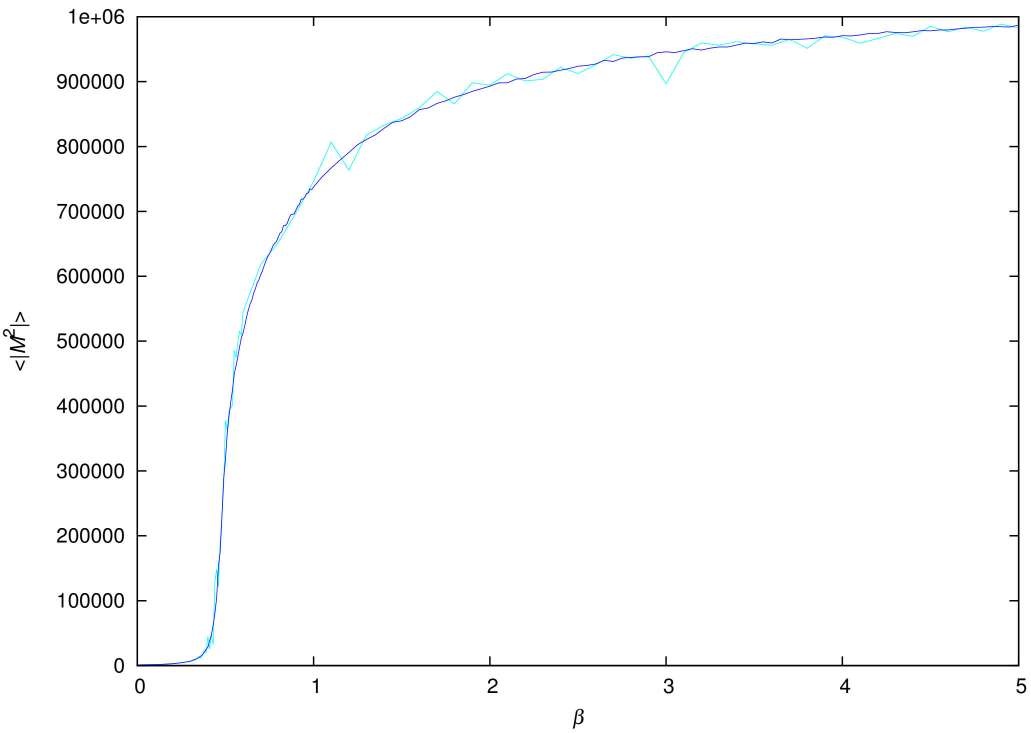

Figure 1: $\langle |M|^2 \rangle$ against β. The difference between the two plots is the number of iterations of the Metropolis algorithm performed for each value of β. The lower resolution curve was iterated 10000 times, whilst the smooth curve underwent 100000 iterations, both in Metropolising the lattice and in evaluating $\langle |M|^2 \rangle$.

Accordingly, there exists a stable low temperature configuration of quasi-long range order. This is assured by the Mermin–Wagner theorem which precludes the existence of Goldstone modes disrupting this order.

At higher energies, the system takes on another state of disordered spins. The transition between these two states is the Kosterlitz–Thouless transition.

The total magnetisation M is determined by the orientation of the spins,

$$M = \sum_{\mathbf{x} \in \Lambda} \sigma_{\mathbf{x}}.$$

Note that by this definition, $M \in \mathbb{C}$. As inhabitants of the (real-valued) macroscopic world, we are interested in the expectation value $\langle |M|^2 \rangle$. In general, for any observable O depending on θ,

$$\langle O \rangle = \frac{1}{Z} \int_{-\pi}^{\pi} \prod_{\mathbf{x} \in \Lambda} d\theta_{\mathbf{x}}\, O(\theta) e^{-\beta S(\theta)}, \tag{3.1}$$

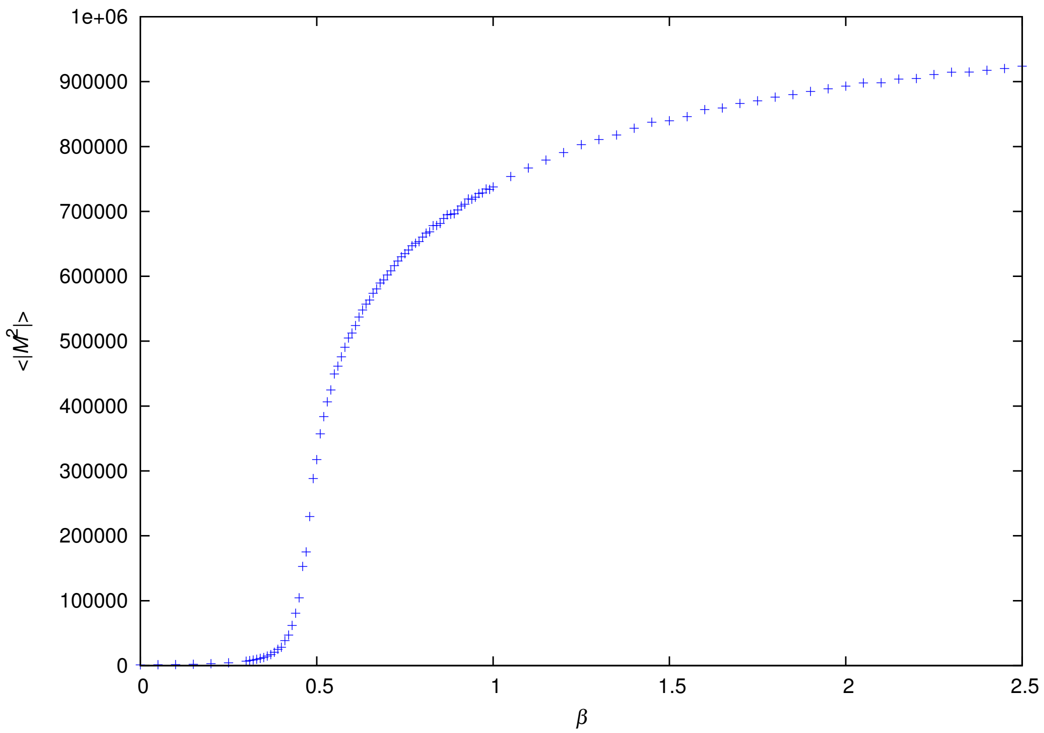

Figure 2: This is the smooth curve plotted in figure 1 with points instead of lines for clarity. For $\beta \in [0.3, 1]$, the resolution was increased from increments of 0.05 to increments of 0.01 in order to better observe the Kosterlitz–Thouless transition whilst not allocating large computer resources to less interesting regions.

where the partition function Z serves as a normalising factor and is given by

$$Z = \int_{-\pi}^{\pi} \prod_{\mathbf{x}\in\Lambda} d\theta_{\mathbf{x}}\, e^{-\beta S(\theta)}. \tag{3.2}$$

Therefore, by (3.1) the expectation value of the observable $|M|^2$ is

$$\begin{aligned} \langle |M|^2 \rangle &= \frac{1}{Z} \int_{-\pi}^{\pi} \prod_{\mathbf{x}\in\Lambda} d\theta_{\mathbf{x}}\, |M|^2 e^{-\beta S(\theta)} \\ &= \frac{1}{Z} \int_{-\pi}^{\pi} \prod_{\mathbf{x}\in\Lambda} d\theta_{\mathbf{x}} \left| \sum_{\mathbf{x}\in\Lambda} \sigma_{\mathbf{x}} \right|^2 e^{-\beta S(\theta)} \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{Z}\left|\sum_{\mathbf{x}\in\Lambda}\sigma_{\mathbf{x}}\right|^2 \int_{-\pi}^{\pi}\prod_{\mathbf{x}\in\Lambda} d\theta_{\mathbf{x}}\, e^{-\beta S(\theta)} \\
&= \left|\sum_{\mathbf{x}\in\Lambda}\sigma_{\mathbf{x}}\right|^2. \qquad (3.3)
\end{aligned}
$$

As an aside, consider a complex variable $z \in \mathbb{C}$. Any such z may be written as $z = x + iy$, so

$$
\begin{aligned}
|z|^2 &= |z\bar{z}| \\
&= (x+iy)(x-iy) \\
&= x^2 + y^2.
\end{aligned}
$$

Therefore, by (3.3) we can write

$$
\begin{aligned}
\langle |M|^2 \rangle &= \left(\sum_{\mathbf{x}} \Re(\sigma_{\mathbf{x}})\right)^2 + \left(\sum_{\mathbf{x}} \Im(\sigma_{\mathbf{x}})\right)^2 \\
&= \left(\sum_{\mathbf{x}} \cos(\theta_{\mathbf{x}})\right)^2 + \left(\sum_{\mathbf{x}} \sin(\theta_{\mathbf{x}})\right)^2.
\end{aligned}
$$

In this manner, $\langle |M|^2 \rangle$ was computed over an energy region of $\beta \in [0,5]$. It is in this region that the elusive Kosterlitz–Thouless transition was observed.

In figure 1 we can clearly see the Kosterlitz–Thouless transition as a steep curve from low magnetisation to large magnetisation as β increases. It occurs in the region of $\beta \approx 0.5, 0.6$. The variations in the lighter curve represent statistical uncertainty and arose because the system had not "settled down" sufficiently. This was accounted for in the smooth curve, which was afforded more time (much of the night) by increasing the number of Metropolis iterations.

In order to reduce on the computational expense, the resolution in β, i.e. how small the increment in β is per iteration, was variable depending on which region it was in. Indeed, as the configuration enters the Kosterlitz–Thouless transition, β increases in value by 0.01 per iteration in order to view the transition with more accuracy. As the system leaves the transition and enters its new topology, the β-increment returns to its relaxed value of 0.05. This is illustrated in figure 2.

In all results, Λ should be taken as a $(32,32)$ lattice.

4 The Two-Point Correlation Function

The correlation between spins on neighbouring lattice sites is described by

$$
C(d) = \sum_{\mathbf{x}\in\Lambda} \cos(\theta_{\mathbf{x}} - \theta_{\mathbf{x}+d\mathbf{e}_x})
$$

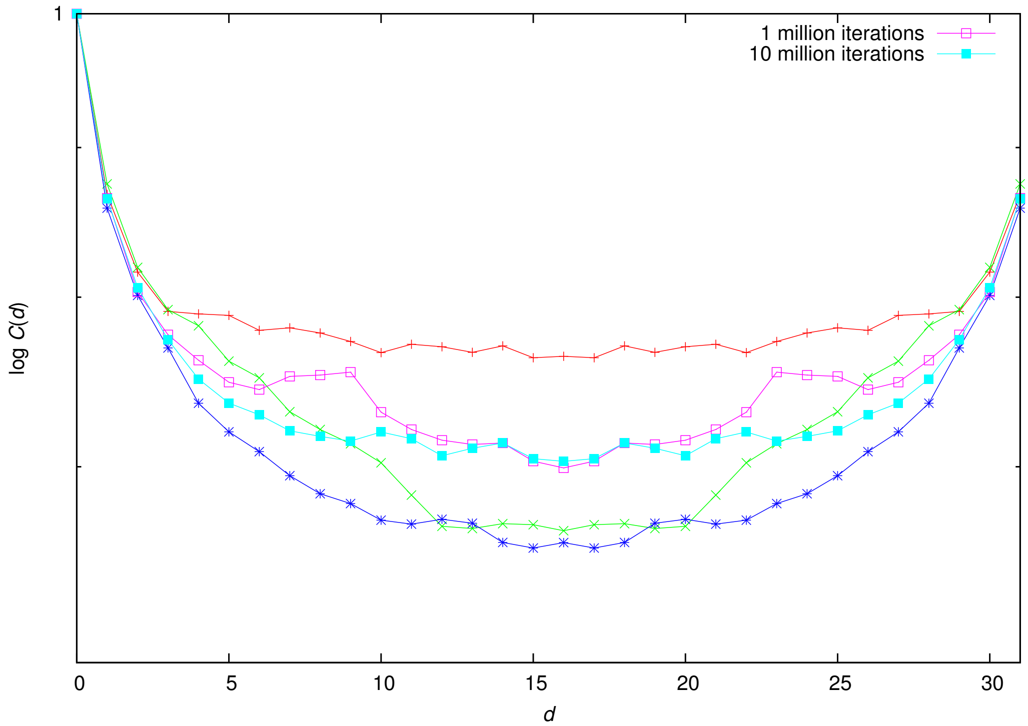

Figure 3: $\log(C(d))$ against d. The different plots emphasise the dependence of the system on stochastic variables. Three of the plots are the result of iterating the Metropolis algorithm 100000 times, one from an iteration of 1 million and one from 10 million. As we expect, the 10 million curve is roughly the average of the others.

for separation in the x-direction, where $\mathbf{e}_x = (1,0)$ and $d \in \mathbb{Z}$. The behaviour of this function changes depending on which side of the KT singularity one finds oneself. In the quasi-long range ordered phase (high β), the correlation function decays as a power law, whereas in the disordered phase (low β) it decays as an exponential.

The correlation function $C(d)$ is plotted logarithmically against d for $\beta = 1$ in figure 3. In this graph, $d = 0$ refers to the correlation of a lattice site with itself. Thus, $C(d)$ was normalised such that $C(0) = 1$. As the lattice is periodic, $C(32) = C(0)$. This is why we expect the correlation function to be symmetric. Indeed, $C(d)$ is symmetric about $d = 16$, the centre of the lattice.

5 Tarball

The following files are contained in the tarball `Fionn_Fitzmaurice_XY.tgz`.

1. `xy.cpp`. This is the source code used to generate all the data in this report (see item 2). The `main` function, aside from initialising the lattice, consists of three separate entities. Each of these corresponds to §§2–4 respectively.

2. `xy.pdf`. "XY", i.e. this document, corresponding to §§1–5.