AQTIVATE

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**The XY Model**

As an example problem in which very high dimensional integrals can be solved by Monte-Carlo methods, we consider the "XY model".

The degrees of freedom of the model are microscopical magnetic moments or "spins". Each spin is a two dimensional vector with length one, that can be parameterized by an angle $\theta \in [0, 2\pi)$,

$$\vec{s} = \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} .$$

One such spin lives on every site $\vec{x}$ of a $D$ dimensional crystal,

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{pmatrix} , \qquad x_i \in \{1, 2, \ldots, L\}.$$

Every site can have a different spin angle $\theta(\vec{x})$. The collection of all spin angles is called a "spin configuration" and will be abbreviated by $\vec{\theta}$. The energy of a spin configuration is given by

$$H(\vec{\theta}) = - \sum_{x_1,\ldots,x_D=1}^{L} \sum_{\mu=1}^{D} \vec{s}(\vec{x}) \cdot \vec{s}(\vec{x} + \hat{\mu}) \, . \tag{1}$$

Here $\hat{\mu}$ denotes a unit vector in direction $\mu$, so the summation is over all pairs of nearest neighbors on the crystal lattice, often written as $\sum_{<\vec{x},\vec{y}>} \vec{s}_x \cdot \vec{s}_y$. Each term contributes the dot-product of the two neighboring spins. The configuration with minimal energy is the one in which all spins are parallel to each other.

Observables in the $XY$ model are computed as expectation values with respect to the PDF $p$,

$$\langle \mathcal{O}(\vec{\theta}) \rangle = \int_0^{2\pi} d^{L^D}\theta \;\; p(\vec{\theta}) \, \mathcal{O}(\vec{\theta}) \, , \tag{2}$$

where $p(\vec{\theta}) = \frac{1}{Z} \exp(-\beta H(\vec{\theta}))$ is the PDF, $Z$ a normalization factor such that $\langle 1 \rangle = 1$, and the parameter $\beta$ is the inverse temperature of the system.

In $D = 2$ dimensions the XY model undergoes a very interesting phase transition at $\beta = \beta_c$, which separates a high temperature "vortex phase" and a low

temperature "spin wave phase". This "Kosterlitz-Thouless" transition is of infinite order and can be observed in several physical systems, e.g. in thin disordered superconducting granular films. The theoretical understanding of the KT transition was awarded with the Nobel price in physics in 2016.

Instead of many millions of atoms, that a real crystal has, we will consider only a few hundred/thousand. To keep the unrealistic boundary effects to a minimum, we will use periodic boundary conditions, which means that the first and last atoms in each direction are by definition nearest neighbors, $x_\mu = L \Rightarrow x_\mu + 1 = 1$ etc.

Some possible observables are

- Internal energy
$$\langle H(\vec{\theta}) \rangle \tag{3}$$
- Magnetization
$$M = \left\langle \frac{1}{L^D} \left\| \sum_{\vec{x}} \vec{s}(\vec{x}) \right\| \right\rangle \tag{4}$$
- Magnetic susceptibility
$$\chi = \left\langle \frac{1}{L^D} \sum_{\vec{x}} \sum_{\vec{y}} \vec{s}(\vec{x}) \cdot \vec{s}(\vec{y}) \right\rangle . \tag{5}$$
- Slice correlation function
$$G(t) = \frac{1}{L} \left\langle \sum_{x_1=1}^{L} \vec{S}(x_1) \cdot \vec{S}(x_1 + t) \right\rangle , \tag{6}$$
where "slice spins" are averages over slices with fixed $x_1$
$$\vec{S}(x_1) = \frac{1}{L^{D-1}} \sum_{x_2,\ldots,x_D=1}^{L} \vec{s}\,(\vec{x}) \ . \tag{7}$$

**Lattice Geometry**
A unique linear or "lexicographical" index of a site $\vec{x}$ can be defined as

$$l = x_1 + L(x_2 - 1) + L^2(x_3 - 1) + \ldots + L^{D-1}(x_D - 1)\,. \tag{8}$$

Using such indices allows to write programs in which the number of dimensions (2 for us) can be arbitrary. Also multi dimensional arrays are avoided. In the "vanilla code" transition between lexicographical indices $l$ and coordinates $x_i$ is done with the functions `lexic` and `alexic`. The function `hop` returns a matrix $h$ with neighborhood relations on the torus, such that $h_{l,\mu}$ is the index of the positive neighbor of site $l$ in direction $\mu$. Values $\mu = D + 1, \ldots 2D$ give the negative neighbors.

**Cluster Algorithm**
The provided code simulates the XY model using a Metropolis algorithm, where spins are proposed to be rotated by a random amount, one at a time, and the proposals are accepted or rejected based on an acceptance probability which can be computed using only spins in the neighborhood of the one to be rotated. The main goal of this project is to implement Ulli Wolff's single cluster algorithm, as described in [1, 2]. The updates are non-local and almost completely eliminate the problem of critical slowing down. The procedure is the following:

1. A direction in the $XY$ plane is chosen randomly. It is represented by the unit vector $\vec{r}$

2. One site $\vec{x}$ is chosen randomly from the lattice and added to the cluster $\mathcal{C}$.

3. All neighbors $\vec{y}$ of $\vec{x}$ are added to the cluster $\mathcal{C}$ with the probability $p_{\vec{r}}(\vec{s}_x, \vec{s}_y) = 1 - e^{\min[0,\, -2\beta \vec{s}_x \cdot \vec{r}\ \vec{s}_y \cdot r]}$ and $\vec{x}$ is marked as "already processed".

4. Step three is repeated recursively for all $\vec{x} \in \mathcal{C}$, that are not marked as "already processed".

5. Finally the system is updated. On all sites belonging to the cluster, the associated spin is reflected on the plane perpendicular to $\vec{r}$:

$$\vec{s}_x\,' = \begin{cases} \vec{s}_x - 2(\vec{s}_x \cdot \vec{r})\vec{r} & x \in \mathcal{C} \\ \vec{s}_x & x \notin \mathcal{C} \end{cases} \tag{9}$$

This algorithm is ergodic, because at least one site is updated and the initial site is selected randomly. A proof of detailed balance can be found in the literature.

**Directions to Explore**
Once the algorithm is working correctly and reproduces known results from literature, I would suggest to investigate the reduction of "critical slowing down".

In the high temperature phase (low $\beta$) of the XY model, the correlation function is expected to decay exponentially

$$\langle G(t) \rangle \sim e^{-t/\xi} \,, \tag{10}$$

for $1 \ll t \ll L/2$. The "correlation length" $\xi$ depends on the inverse temperature $\beta$ and diverges as the Kosterlitz-Thouless transition ($\beta_c \approx 1.1199$) is approached

$$\begin{aligned} \xi &= A \, \exp\left( C \left| \frac{\beta_c - \beta}{\beta_c} \right|^{-\frac{1}{2}} \right) \,, \\ A &= 0.233 \pm 0.003 \,, \\ C &= 1.776 \pm 0.004 \,. \end{aligned} \tag{11}$$

Metropolis algorithms are suffering from critical slowing down, i.e. autocorrelations diverge as $\tau \sim \xi^z$, with a dynamical critical exponent $z$, which is $\approx 2$ for algorithms with local updates. What $z$ do you observe with your cluster algorithm?

# References


[1] U. Wolff, "Collective Monte Carlo Updating for Spin Systems," Phys. Rev. Lett. **62** (1989), 361

[2] U. Wolff, "Collective Monte Carlo Updating in a High Precision Study of the X-y Model," Nucl. Phys. B **322** (1989), 759-774