CS-294 and Stat-260: Spin Systems **Spring 2003**

Lecture 1: January 22

Lecturer: Fabio Martinelli *Scribes: Gábor Pete*

1.1 Useful readings

On the course webpage you can find several resources. The main textbooks are the following:

1. Wei-Shih Yang: Mathematical Methods in Statistical mechanics. These are really condensed, and useful in general.
2. Barry Simon: The statistical mechanics of lattice gases. Not an easy mathematics text, but also contains good accounts of some nice combinatorial topics.
3. Frank Harary (Ed.): Graph Theory and Theoretical Physics. We will use Kasteleyn's paper on planar Ising models and counting matchings.
4. Fabio Martinelli: Lectures on Glauber Dynamics for discrete spin models. This is for the MCMC approach. Can be found on the web.

1.2 The Ising model

The Ising model is the simplest and most famous spin system model to study phase transitions. It was introduced in 1925 by Ernst Ising in his Ph.D. thesis. He solved the model completely for **Z**, and found that no phase transition occurs. He concluded that this should be the case for all dimensions — a fatal mistake. Inspite of this, the model was renamed after him, but English speakers usually mispronounce his name — a revenge of history.

1.2.1 Basic definitions

Let $G = (V, E)$ be a finite graph, and call $\Omega = \{-1, +1\}^V$ the state space, with elements $\sigma = \{\sigma_x\}_{x\in V}$. The variable $\sigma_x \in \{-1, +1\}$ is called the spin at vertex x. This is a **spin system**. Sometimes the variables $\rho_x \in \{0, 1\}$ are used: in this case $\rho_x = 1$ interpreted as having a particle at the site x, and $\rho_x = 0$ means a vacant site. Then the system is called a **lattice gas model**.

There is an **energy functional** defined on Ω. For the Ising model this functional is defined as

$$H(\sigma) = -J\Sigma_{(x,y)\in E}\sigma_x\sigma_y, \tag{1.1}$$

where J is a real constant, the **interaction strength**. Note that $H(\sigma)$ is built up from the local energy terms $-J\sigma_x\sigma_y$, i.e. our model is defined by nearest-neighbour interactions. Now we introduce the **inverse**

temperature parameter $\beta \sim 1/T$, and consider the following probability measure on Ω:

$$\mu(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta}, \qquad Z_\beta = \sum_{\sigma\in\Omega} e^{-\beta H(\sigma)}. \tag{1.2}$$

This Z_β is called the **partition function**, and, as usually generating functions do, contains basically all information about the system. Clearly, the main problem we are interested in is to understand $\mu = \mu_\beta$, called the **Gibbs measure** (we will see later what "Gibbsian" means). First of all note that for $J > 0$, which is called the **ferromagnetic case**, the minimum of $H(\sigma)$ and so the maximum of $\mu(\sigma)$ are attained at $\sigma \equiv$ const. More generally, spins like to agree along edges, and for $\beta \to \infty$ the measure concentrates on the two constant configurations. The **antiferromagnetic case** $J < 0$, where neighbouring spins like to differ, is much harder, and we will not consider it on this course.

For any function $f : \Omega \longrightarrow \mathbf{R}$, we can consider the expectation and the variance:

$$\mu(f) = \langle f \rangle = \sum_{\sigma\in\Omega} \mu(\sigma) f(\sigma), \qquad \mathrm{Var}(f) = \mu(f^2) - \mu(f)^2. \tag{1.3}$$

1.2.2 Thermodynamical objects

We are going to define some physics-inspired quantities, which also have clear mathematical importance.

$$\textbf{Free energy}: \quad F(\beta) = -\frac{1}{\beta}\log Z_\beta. \tag{1.4}$$

Note that $Z_\beta = e^{-\beta F(\beta)}$ and $\frac{d}{d\beta}F(\beta) = \mu(H)$.

$$\textbf{Specific heat}: \quad C(\beta) = \frac{d}{d(1/\beta)}\mu(H) = -\beta^2 \frac{d^2}{d\beta^2}F(\beta). \tag{1.5}$$

The "specific heat" is the amount of heat you have to provide to increase the temperature of one kg of material by 1 Celsius degree. In our case it is related to the fluctuation of the system: $C(\beta) = \beta^2 \mathrm{Var}(H)$.

Now we modify our $H(\sigma)$ by introducing an **external magnetic field**:

$$H(\sigma, h) = -J \sum_{(x,y)\in E} \sigma_x \sigma_y - \sum_{x\in V} h_x \sigma_x, \tag{1.6}$$

where $h_x \in \mathbf{R}$; sometimes $h_x \equiv h$ constant. If $h > 0$, then $H(\sigma)$ has a unique minimum at $\sigma \equiv +1$. A very difficult famous problem is the case when the h_x's are i.i.d. random variables.

Now $F(\beta, h) = -\frac{1}{\beta}\log Z(\beta, h)$. This is a nice smooth function for any finite graph G. And we can consider

$$\textbf{Magnetization}: \quad M(\beta, h) = \frac{1}{|V|}\sum_{x\in V}\mu(\sigma_x) = -\frac{1}{|V|}\frac{\partial}{\partial h}F(\beta, h). \tag{1.7}$$

Furthermore,

$$\frac{1}{\beta|V|}\frac{\partial}{\partial h}M(\beta, h) = \mathrm{Var}\left(\frac{1}{|V|}\sum_{x\in V}\sigma_x\right). \tag{1.8}$$

For $h = 0$ we have $\mu(\sigma_x) = 0$ for all $x \in V$, by symmetry between the spins ± 1, so $M(\beta, 0) = 0$. Clearly, $M(\beta, h)$ is monotone increasing in h, and $M(\beta, h) \to \mathrm{sgn}(h)$ as $\beta \to \infty$, i.e. as the interactions are getting infinitely strong.

1.2.3 Is there a phase transition?

Now the main question of the field is if the above discontinuity can happen already for finite β if the underlying graph G is infinite. More precisely, take an infinite graph, and a "nice" exhaustion of it by finite subgraphs, for example $V_\ell = \{\underline{x} \in \mathbf{Z}^\nu, |x_i| \leq \ell\}$, $\ell \to \infty$. Is there a finite β for which

$$\lim_{h\to 0-}\lim_{\ell\to\infty} M_\ell(\beta,h) < 0 < \lim_{h\to 0+}\lim_{\ell\to\infty} M_\ell(\beta,h)? \tag{1.9}$$

The implication of such a discontinuity **(a first order phase transition)** for the infinite graph would be the following. The sequence of probability measures $\mu_\ell(\beta)$ has of course some accumulation points. For $h \neq 0$ there should always be only one accumulation point, with $\mathrm{sgn}(M(\beta,h)) = \mathrm{sgn}(h)$. But for $h = 0$ it might happen that we have a limit measure with $M_+(\beta,0) > 0$ and another with $M_-(\beta,0) < 0$. That is, we might have multiple "equilibrium measures", and **spontaneous magnetization** happens. We will prove that for $\nu \geq 2$ there exists $0 < \beta_c(\mathbf{Z}^\nu) < \infty$ such that this happens for all $\beta > \beta_c$, and doesn't happen for $\beta < \beta_c(\mathbf{Z}^\nu)$.

1.2.4 Translation to the Lattice Gas Model

Recall we have $\rho_x \in \{0,1\}$. Now the energy function is

$$H(\rho,\lambda) = K\sum_{(x,y)\in E}\rho_x\rho_y - \lambda\sum_{x\in V}\rho_x, \tag{1.10}$$

with $K > 0$, and where $\lambda \in \mathbf{R}$ is called the **chemical potential**. The partition function $Z(\beta,\lambda)$ is defined appropriately. Substituting $\sigma_x = 2\rho_x - 1$ we get

$$H(\rho) = -J\sum_{(x,y)\in E}\sigma_x\sigma_y - \sum_{x\in V} h_x\sigma_x + C, \tag{1.11}$$

with $J = K/4$, $h_x = \frac{\lambda}{2} + \frac{K}{4}\deg(x)$. So we get the Ising model with magnetic field h_x; moreover, for a regular graph G we have $h_x \equiv \mathrm{const}$.

1.2.5 High level problems

The main questions to be answered are the following.

1. Try to compute $Z(\beta,h)$. Then we have $F(\beta,h)$ and $M(\beta,h)$, so we have basically everything. This is possible only for subgraphs of $\mathbf{Z}$, and for planar graphs with $h = 0$ — we will see the nice combinatorial approach of Kasteleyn.

2. When there is no explicit computation: try to approximate $Z(\beta,h)$, e.g. by a power series expansion.

3. MCMC sampling from the Gibbs measure μ, to understand the measure.

Answering these questions would of course also provide different approaches to understand phase transition phenomena. For example, what is the physical relevance of different mixing times of the Gibbs sampler Markov chain for different β values?

1.2.6 Some related areas

The first application is to **image reconstrucion**. Consider a black-and-white "true image", with pixels $\{\sigma_x\}_{x \in V}$. But we have an "actual image" $\eta_x = \sigma_x + \xi_x$ with noises ξ_x i.i.d. Normal$(0, \delta^2)$ random variables. Assume that the true image is coming from a measure of the form $\mu(\sigma) = \frac{1}{Z} e^{-\beta H(\sigma)}$. The energy function $H(\sigma)$ can be the one corresponding to the Ising model, but one can also cook more realistic ones, e.g. favouring straight lines in the image. Now we want to compute

$$\Pr(\sigma|\eta) \sim e^{-\beta H(\sigma) + \delta^{-2} \sum_x \eta_x \delta_x}. \tag{1.12}$$

Note that $\delta \to 0$ yields $\Pr(\sigma|\eta) \to \mu(\sigma)$.

Another related area of research is called **broadcasting over a noisy channel in a tree network**. Given the original information $\sigma_r \in \{\pm 1\}$ at the root r of a tree T, we broadcast spins through edges with a flipping probability $\epsilon \in [0, 1/2)$. A brief computation shows that the random configuration of spins at all the vertices of the tree is just the Ising model with

$$\frac{\epsilon}{1 - \epsilon} = e^{-2\beta J}. \tag{1.13}$$

The phase transition question here is the following: given the tree T, how large ϵ can be that still allows us to reconstruct σ_r with probability bigger than the trivial 1/2, if we can see the spins only at the leaves? We will see similar **decay of information** questions later on the course.