Spin glasses and Stein's method

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Spin glasses

- Magnetic materials with strange behavior.
- Not explained by ferromagnetic models like the Ising model.
- Theoretically studied since the 70's. An important example: Sherrington-Kirkpatrick model.
- High temperature phase: Thouless-Anderson-Palmer. Low temperature phase: Mézard and Parisi.
- Mathematically almost intractable until the late 90's.
  - Early results due to Aizenman, Lebowitz, Ruelle ('87), Fröhlich and Zegarliński ('87).
  - Notable papers due to Comets and Neveu ('95), Shcherbina ('99) etc.
  - Series of breakthroughs from Talagrand (1998 - present).
  - Groundbreaking contributions from Guerra & Toninelli ('02) and Guerra ('03), taken to completion by Talagrand in 2006.

    The Parisi formula. *Ann. Math. (2)* **163** no 1, 221–263.
  - Still, a lot of mysteries.

The Sherrington-Kirkpatrick model

- N spins. State space: $\Sigma_N = \{-1, 1\}^N$.
- Gibbs measure on Σ_N for the SK model:

$$G_N(\sigma) = Z_N^{-1} \exp\left(\frac{\beta}{\sqrt{N}} \sum_{i<j\leq N} g_{ij}\sigma_i\sigma_j + h \sum_{i\leq N} \sigma_i \right)$$

  where
  - $(g_{ij})_{i<j\leq N}$ is a fixed realization of independent standard gaussian random variables (the disorder),
  - β and h are parameters,
  - Z_N is the normalizing constant (partition function).
- Notation:

$$\langle f(\sigma) \rangle := \sum_{\sigma\in\Sigma_N} f(\sigma) G_N(\sigma).$$

High temperature phase

- Let z be a standard gaussian r.v. Then

$$\lim_{N\to\infty} \frac{\log Z_N}{N} = \log 2 + \mathbb{E}\log\cosh(\beta z\sqrt{q} + h) + \frac{\beta^2}{4}(1-q)^2,$$

where q is determined by

$$q = \mathbb{E}\tanh^2(\beta z\sqrt{q} + h).$$

Rigorously proven to hold for $\beta < 1/2$, all h (Talagrand).

- Conjectured description of the full high temperature regime: All (β, h) such that

$$\beta^2 \mathbb{E}\frac{1}{\cosh^4(\beta z\sqrt{q} + h)} < 1.$$

The line where equality holds is called the Almeida-Thouless line.

The Gibbs measure at high temperature

- Spins are approximately independent, i.e. with high probability,

$$\langle \sigma_{i_1} \sigma_{i_2} \cdots \sigma_{i_k} \rangle \approx \langle \sigma_{i_1} \rangle \langle \sigma_{i_2} \rangle \cdots \langle \sigma_{i_k} \rangle.$$

  This is a deep fact and surprisingly hard to prove. Both sides are nondegenerate random variables in the limit.

- Moreover, $\langle \sigma_{i_1} \rangle, \ldots, \langle \sigma_{i_k} \rangle$ are approximately i.i.d.
- First proved by Talagrand using his cavity argument.
- If $h = 0$, then $\langle \sigma_i \rangle \equiv 0$ for all i.
- What if $h \neq 0$? No simple formulas for $\langle \sigma_1 \rangle, \ldots, \langle \sigma_N \rangle$.

The TAP equations

When $(\beta, h) \in$ the high temperature regime, the random quantities $\langle \sigma_1 \rangle, \ldots, \langle \sigma_N \rangle$ satisfy

$$\langle \sigma_i \rangle \approx \tanh\biggl(\frac{\beta}{\sqrt{N}} \sum_{j \neq i} g_{ij} \langle \sigma_j \rangle + h - \beta^2 (1-q) \langle \sigma_i \rangle \biggr),$$

where q solves $q = \mathbb{E} \tanh^2(\beta z \sqrt{q} + h)$, z being a standard gaussian r.v.

- Discovered by Thouless, Anderson, and Palmer ('77).
- Rigorous proof by Talagrand ('03) using the cavity method.
- Unique solution if β is smaller than a constant.
- Talagrand also shows that $\langle \sigma_i \rangle$ converges in law to $\tanh(\beta z \sqrt{q} + h)$.

The cavity method

- Basically, a very complex induction over N.
- Coefficient of σ_N in the Hamiltonian is

$$\frac{\beta}{\sqrt{N}} \sum_{j=1}^{N-1} g_{Nj}\sigma_j + h.$$

- Replace this by an independent gaussian r.v. to get a new Hamiltonian.
- Determine the mean and variance of this r.v. such that the annealed measures remain 'approximately the same'.
- Using gaussian interpolation and a certain recursive argument, Talagrand shows that it is possible to do this if β is sufficiently small. This is the foundation of the cavity induction.
- We will follow a different route, starting from the next slide.

Explaining the TAP equations: (I) Local fields

- Local field at site i:

$$\ell_i = \frac{1}{\sqrt{N}} \sum_{j \neq i} g_{ij} \sigma_j.$$

- Easy to show: The conditional expectation of σ_i given $(\sigma_j)_{j \neq i}$ is exactly $\tanh(\beta \ell_i + h)$.
- This gives the equations

$$\langle \sigma_i \rangle = \langle \tanh(\beta \ell_i + h) \rangle.$$

- Thus, if we knew the limiting distribution of ℓ_i, $\langle \sigma_i \rangle$ could be computed directly. But this was not known previously.

Explaining the TAP equations: (II) The Onsager correction

- If X is a random variable with small variance, then

$$\mathbb{E}\tanh(aX + b) \approx \tanh(a\mathbb{E}(X) + b).$$

This is the usual mean-field approximation.

- Applying the naïve mean-field logic (although $\mathrm{Var}(\ell_i) \not\to 0$), we may wonder whether

$$\begin{aligned}\langle\sigma_i\rangle = \langle\tanh(\beta\ell_i + h)\rangle &\overset{?}{\approx} \tanh\big(\beta\langle\ell_i\rangle + h\big)\\ &= \tanh\bigg(\frac{\beta}{\sqrt{N}}\sum_{j\neq i} g_{ij}\langle\sigma_j\rangle + h\bigg).\end{aligned}$$

Not surprisingly, this is incorrect.

- In the TAP equations, we have

$$\langle\sigma_i\rangle \approx \tanh\bigg(\frac{\beta}{\sqrt{N}}\sum_{j\neq i} g_{ij}\langle\sigma_j\rangle + h - \beta^2(1-q)\langle\sigma_i\rangle\bigg).$$

The extra term is called the Onsager correction term in physics.

Onsager correction and mixture gaussians

- Let ϕ_{μ,σ^2} be the gaussian density with mean μ and variance σ^2. Let $\psi_{p,\mu_1,\mu_2,\sigma^2}$ be the mixture gaussian density

$$\psi_{p,\mu_1,\mu_2,\sigma^2} = p\phi_{\mu_1,\sigma^2} + (1-p)\phi_{\mu_2,\sigma^2}.$$

- Suppose $\mu_2 > \mu_1$, and we define

$$a = \frac{\mu_2 - \mu_1}{2\sigma^2}, \ b = \frac{1}{2}\log\frac{p}{1-p} - \frac{\mu_2^2 - \mu_1^2}{4\sigma^2}.$$

  Then, if $X \sim \psi_{p,\mu_1,\mu_2,\sigma^2}$, then

$$\mathbb{E}\tanh(aX + b) = \tanh(a\mathbb{E}(X) + b - (2p-1)a^2\sigma^2).$$

- This is what happens! The local fields have mixture gaussian laws and the highlighted term is the Onsager correction term.

Our main result: Limit law of local fields

- Recall: The local field at site i is defined as

$$\ell_i := \frac{1}{\sqrt{N}} \sum_{j \neq i} g_{ij} \sigma_j.$$

- For each i, let r_i be the random variable

$$r_i := \frac{1}{\sqrt{N}} \sum_{j \neq i} g_{ij} \langle \sigma_j \rangle - \beta(1-q) \langle \sigma_i \rangle.$$

- Let ν_i be the (random) mixture gaussian probability measure with density function

$$p_i \phi_{r_i + \beta(1-q), 1-q} + (1 - p_i) \phi_{r_i - \beta(1-q), 1-q},$$

where

$$p_i = \frac{e^{\beta r_i + h}}{e^{\beta r_i + h} + e^{-\beta r_i - h}}.$$

- Under the Gibbs measure, ν_i approximates the law of ℓ_i for large N.

Our main result: Limit law of local fields

Theorem

Suppose (β, h) is in the high temperature regime and q satisfies

$$q = \mathbb{E}\tanh^2(\beta z\sqrt{q} + h),$$

where z is a standard gaussian r.v. Let $\ell_1, \ldots, \ell_N$ be the local fields and let $\nu_1, \ldots, \nu_N$ be defined as in the previous slide. Then for any bounded measurable $f : \mathbb{R} \to \mathbb{R}$ and any $1 \le i \le N$, we have

$$\mathbb{E}\left(\langle f(\ell_i)\rangle - \int_{\mathbb{R}} f(x)\nu_i(dx)\right)^2 \le \frac{C(\beta, h)\|f\|_\infty^2}{\sqrt{N}},$$

where $C(\beta, h)$ is a constant depending only on β and h.

- Recall: $\langle \sigma_i \rangle = \langle \tanh(\beta\ell_i + h)\rangle$. Taking $f(x) = \tanh(\beta x + h)$, the TAP equations follow easily.
- Proof is by Stein's method.

Stein's method

- Let X and Z be two random variables. Suppose we want to show that they approximately have the same distribution.
- Basic steps in Stein's method:
  1. Identify an operator T such that for all functions h,

     $$\mathbb{E}\big(Th(Z)\big) = 0.$$

     (T is called a Stein characterizing operator.) For example, if Z is standard gaussian, then $Th(x) = h'(x) - xh(x)$ is a characterizing operator.
  2. Given a function f, find h such that

     $$Th(x) = f(x) - \mathbb{E}(f(Z)).$$

     Relate the properties of h to those of f.
  3. By the definition of h it follows that

     $$|\mathbb{E}f(X) - \mathbb{E}f(Z)| = |\mathbb{E}(Th(X))|.$$

     Compute a bound on $|\mathbb{E}(Th(X))|$ by whatever means possible.

Stein's method for gaussian approximation

- Let Z be a standard gaussian r.v. Then for all h,

$$\mathbb{E}(h'(Z) - Zh(Z)) = 0.$$

Thus, $Th(x) := h'(x) - xh(x)$ is a characterizing operator for the standard gaussian distribution.

- Thus, to show that a r.v. W is approximately standard gaussian, one has to show that for all h,

$$\mathbb{E}(h'(W) - Wh(W)) \approx 0.$$

Stein's method for mixture gaussians

- For the mixture gaussian density

$$p\phi_{\mu_1,\sigma^2} + (1-p)\phi_{\mu_2,\sigma^2}$$

the characterizing operator is

$$Th(x) = h'(x) - \left(\frac{x-\mu}{\sigma^2} - a\cdot \tanh(ax+b)\right)h(x),$$

where μ, a, b are defined as

$$\mu = \frac{\mu_1+\mu_2}{2}, \quad a = \frac{\mu_2-\mu_1}{2\sigma^2},$$
$$b = \frac{1}{2}\log\frac{p}{1-p} - \frac{\mu_2^2-\mu_1^2}{4\sigma^2}.$$

- Appears to be naturally connected to physical models. Does not occur in the literature on Stein's method.

The Approximation Lemma

Lemma

Suppose $g = (g_1, \ldots, g_n)$ is a collection of independent standard gaussian random variables, and $h_1, \ldots, h_n$ are absolutely continuous functions of g. Then

$$\mathbb{E}\biggl(\sum_{i=1}^n g_i h_i - \sum_{i=1}^n \frac{\partial h_i}{\partial g_i}\biggr)^2 = \sum_{i=1}^n \mathbb{E}(h_i^2) + \sum_{i,j=1}^n \mathbb{E}\biggl(\frac{\partial h_i}{\partial g_j}\frac{\partial h_j}{\partial g_i}\biggr).$$

Idea: If the right hand side is small, then the lemma 'generates' the equation

$$\sum_{i=1}^n g_i h_i \approx \sum_{i=1}^n \frac{\partial h_i}{\partial g_i}.$$

Can be used to obtain Stein characterizing equations for highly complex functions of gaussian random variables.

Example

- Consider the SK model with zero external field (the simple case):

$$G_N(\sigma) = Z_N^{-1} \exp\left(\frac{\beta}{\sqrt{N}} \sum_{i<j\leq N} g_{ij}\sigma_i\sigma_j\right).$$

- We wish to generate a characterizing equation for the local field at site 1:

$$\ell_1 = \frac{1}{\sqrt{N}} \sum_{j=2}^{N} g_{1j}\sigma_j.$$

- Fix a smooth function f. For each $j = 2, \ldots, N$, let

$$h_j = \frac{1}{\sqrt{N}} \big\langle \sigma_j f(\ell_1) \big\rangle.$$

- Then

$$\sum_{j=2}^{N} g_{1j} h_j = \big\langle \ell_1 f(\ell_1) \big\rangle.$$

Example contd.

- On the other hand, an easy computation gives

$$\frac{\partial h_j}{\partial g_{1j}} = \frac{\langle f'(\ell_1)\rangle + \beta\langle \sigma_1 f(\ell_1)\rangle - \beta\langle \sigma_j f(\ell_1)\rangle\langle \sigma_1\sigma_j\rangle}{N}.$$

- The 2nd term. Note that ℓ_1 does not depend on σ_1, and the conditional expectation of σ_1 given $\sigma_2, \ldots, \sigma_N$ is $\tanh(\beta\ell_1)$. Thus,

$$\langle \sigma_1 f(\ell_1)\rangle = \langle \tanh(\beta\ell_1) f(\ell_1)\rangle.$$

- The 3rd term. It follows from the high temperature theory for $\beta < 1$ that for $2 \le j \le N$,

$$\langle \sigma_1\sigma_j\rangle \approx \langle \sigma_1\rangle\langle \sigma_j\rangle = 0.$$

Example contd.

- Thus, if we can apply the Approximation Lemma, we get the approximation

$$\sum_{j=2}^{N} g_{1j} h_j \approx \sum_{j=2}^{N} \frac{\partial h_j}{\partial g_{1j}}$$

which is equivalent to

$$\left\langle \ell_1 f(\ell_1) - f'(\ell_1) - \beta \tanh(\beta \ell_1) f(\ell_1) \right\rangle \approx 0.$$

- Now, the operator

$$Tf(x) = xf(x) - f'(x) - \beta \tanh(\beta x) f(x)$$

is a Stein characterizing operator for the mixture gaussian density

$$\tfrac{1}{2}\phi_{\beta,1} + \tfrac{1}{2}\phi_{-\beta,1}.$$

- This procedure 'discovers' the limiting distribution of ℓ_1.

When $h \neq 0$

- When $h \neq 0$, ℓ_1 does not have a nonrandom limiting distribution. The situation becomes more complex.
- Given a function u, we start with a solution $f(x, y)$ of the p.d.e.

$$\frac{\partial f}{\partial x}(x,y) - \left(\frac{x-y}{\sigma^2} - \beta \tanh(\beta x + h)\right) f(x,y)$$
$$= u(x) - \int_{\mathbb{R}} u(t) \frac{\cosh(\beta t + h) e^{-\frac{(t-y)^2}{2(1-q)}}}{\sqrt{2\pi(1-q)}\cosh(\beta\mu + h) e^{\frac{1}{2}\beta^2(1-q)}} dt.$$

- Then, defining

$$r_1 = \frac{1}{\sqrt{N}} \sum_{j=2}^{N} g_{1j} \langle \sigma_j \rangle - \beta(1-q)\langle \sigma_1 \rangle,$$

  we let

$$h_j = \frac{1}{\sqrt{N}} \big\langle \big(\sigma_j - \langle \sigma_j \rangle\big) f(\ell_1, r_1) \big\rangle.$$

- The proof is completed by an application of the Approximation Lemma with these h_j's.

Distribution of $\langle \sigma_1 \rangle$

- By the TAP equations,

$$\langle \sigma_1 \rangle \approx \tanh(\beta r_1 + h),$$

where

$$r_1 = \frac{1}{\sqrt{N}} \sum_{j=2}^{N} g_{1j} \langle \sigma_j \rangle - \beta(1-q)\langle \sigma_1 \rangle.$$

- Thus, it suffices to find the limiting distribution of r_1.
- Repeatedly integrating by parts, we can get

$$\mathbb{E}(r_1 f(r_1)) \approx q\mathbb{E}\big(f'(r_1)\langle \eta_1 \rangle\big)$$

where

$$\eta_1 = 1 + \frac{\beta \sigma_1}{\sqrt{N}} \sum_{j=2}^{N} g_{1j}\big(\sigma_j - \langle \sigma_j \rangle\big) - \beta^2(1-q)\big(1 - \langle \sigma_1 \rangle^2\big).$$

Distribution of $\langle \sigma_1 \rangle$ contd.

- Applying the Approximation Lemma with

$$h_j = \frac{\beta}{\sqrt{N}}\big(\langle \sigma_1 \sigma_j \rangle - \langle \sigma_1 \rangle \langle \sigma_j \rangle\big),$$

  we can show that $\langle \eta_1 \rangle \approx 1$.

- Combined with the earlier approximation

$$\mathbb{E}(r_1 f(r_1)) \approx q\mathbb{E}\big(f'(r_1)\langle \eta_1 \rangle\big),$$

  this shows that $\mathbb{E}(r_1 f(r_1)) \approx q\mathbb{E}(f'(r_1))$.

- Thus, r_1 is a gaussian r.v. with mean zero and variance q in the large N limit.

Summary and future directions

- Often in spin glasses and other models we have the situation that for some random quantity X,

$$\mathbb{E}\tanh(aX + b) = \tanh(a\mathbb{E}(X) + b + \text{a correction term}).$$

- We show that this happens if the distribution of X is a mixture of two gaussian densities.
- Following this line, we derive the TAP equations for the SK model by showing that the local field is indeed a mixture of two gaussians in the limit.
- Gives total variation error bounds.
- The key tool is the Approximation Lemma that generates characterizing equations for Stein's method.
- The Approximation Lemma can possibly be used to derive/discover limiting distributions of other objects.
- Results apply only to the high temperature phase. Possible to extend to low temperature???