Mechanics - Lecture 13 - 5/2/2018 (pg 13.4 corrected)

Are there alternatives besides (a) exact evaln of integrals, in the simplest settings (eg start of Lecture 12) and (b) numerical soln by Markov chain Monte Carlo (eg rest of Lecture 12)?

Yes: two further alternatives are

- "mean field theory"
  - advantage: relatively elementary
  - disadvantage: gives estimate of uncontrolled validity
- "real space renormalization
  - advantage: relatively systematic
  - disadvantage: more complicated.

Since our time is limited, I'll discuss only mean field theory, following (more or less) Buhler's §3.7-3.8. (For a quick intro to real space renormalization see §5.6 of Chorin + Hald.)

Start by explaining the main idea, which is "variational approxn". If calcns are inconvenient using the real H, we can ask whether there's a simpler H_0 (for which calcns are easier) that provides a good model.

How to assess "goodness" of H_0 as a model? Observe that if Z_0 = partition fn of H_0, Z = partition fn of H, then (using cont's notation)

$$\frac{Z}{Z_0} = \frac{\int e^{-\beta H}}{Z_0} = \frac{\int e^{-\beta(H-H_0)} e^{-\beta H_0}}{Z_0}$$

$$= \langle e^{-\beta(H-H_0)} \rangle_0$$

where $\langle \ \rangle_0$ denotes avg wrt canonical distrn of H_0.

But $e^{-\beta x}$ is a convex fn of x; so by Jensen's inequality

$$e^{-\beta\langle H-H_0\rangle_0} \leq \langle e^{-\beta(H-H_0)} \rangle_0$$

whence

$$\frac{Z}{Z_0} \geq e^{-\beta\langle H-H_0\rangle_0}$$

Writing $Z = e^{-\beta F}$, $Z_0 = e^{-\beta F_0}$, we can write this as

$$F \leq F_0 + \langle H-H_0\rangle_0$$

We usually wouldn't know the LHS. But if we have a family of candidates for H_0, the one that minimizes the RHS is apparently "best".

Example, to show how this works: mean field theory for the 2D Ising model:

$$H = -\frac{1}{2} \sum_{\substack{(i,j) + \\ (i',j') \text{ are} \\ \text{nearest neighbors}}} s_{ij} s_{i'j'} - B \sum s_{ij}$$

(here $s_{ij} = \pm 1$; $1 \le i \le N$ and $1 \le j \le N$; B is an "applied field" which favors $s_{ij} = 1$ if $B > 0$ and $s_{ij} = -1$ if $B < 0$).

I mentioned @ end of Lecture 12 (for $B = 0$, but it's also true for $B \neq 0$) that for low temp (large β) the canonical distn is concentrated near the uniform states (of course for $B > 0$, the part near $s_{ij} \equiv 1$ is more likely).

How does mean field theory work in this case? Use $H_0 = -B^* \sum_{i,j} s_{ij}$. Suppose "best" B^* is $B + \hat{B}$; then quadratic term in H is being mimicked by "mean field" $\hat{B}$.

How to find "best" B^*? I'll do this calcn for $\underline{B=0}$ (Bubler permits any B, but key ideas are already present when $B=0$).

Key pt that makes this computable: in canonical distrn for $H_0 = -B^* \sum s_{ij}$ the spins are <u>independent</u>

<u>step 1</u>: Calculate Z_0. If there were just one spin Z_0 would be $e^{-\beta B^*} + e^{\beta B^*} = 2\cosh(\beta B^*)$. For N^2 indep spins this becomes

$$Z_0 = [2\cosh(\beta B^*)]^{N^2}$$

$$\Rightarrow F_0 = -\frac{1}{\beta} \ln Z_0 = \frac{-N^2}{\beta} \ln(2\cosh(\beta B^*))$$

<u>step 2</u>: Calculate $\langle H - H_0 \rangle_0$; taking $B=0$. This is

$$-\frac{1}{2} \sum_{\text{neighbors}}' \langle s_{ij} s_{i'j'} \rangle_0 - B^* \sum' \langle s_{ij} \rangle_0$$

Since $\{s_{ij}\}$ are indep in canonical distrn for H_0,

$$\langle s_{ij} s_{i'j'} \rangle_0 = \langle s_{ij} \rangle_0^2 .$$

Recall now that $\langle H_0 \rangle_0 = -\frac{\partial}{\partial \beta} \ln Z_0(\beta)$

which becomes

$$-N^2 B^{\#} \langle s_{ij} \rangle_0 = -N^2 \frac{\partial}{\partial \beta} \ln (2\cosh \beta B^{\#})$$

$$\Rightarrow \langle s_{ij} \rangle_0 = -\tanh (\beta B^{\#})$$

So $$\langle H - H_0 \rangle_0 = -2N^2 \left[\tanh (\beta B^{\#})\right]^2 + N^2 B^{\#} \tanh (\beta B^{\#})$$

Thus (cancelling a common factor of N^2) minimization of $F_0 + \langle H - H_0 \rangle_0$ is equiv to

$$\min_{B^{\#}} \; -\frac{1}{\beta} \ln (2\cosh \beta B^{\#}) - 2\left[\tanh (\beta B^{\#})\right]^2 + B^{\#} \tanh (\beta B^{\#}).$$

Deriv vanishes when

$$B^{\#} = 4 \tanh (\beta B^{\#}).$$

If β is large there are 3 solns ($B^{\#} = 0$ + two more); the min is at the nonzero solns (which are equal up to sign).

Since $\langle s_{ij} \rangle_0 = -\tanh (\beta B^{\#})$, we see that the predicted value of $\langle s_{ij} \rangle_0$ is nonzero (with two distinct possible values) when β is large.

(Of course, for Canonical distrn assoc
$H = -\frac{1}{2}\sum' s_{ij} s_{i'j'}$ the canonical distrn is
symmetric abt exchanging +1 and -1, so
$\langle s_{ij} \rangle$ is zero. But nonuniqueness of B^*
reflects the fact that Canonical distrn
consists of two symmetry-related masses,
one near $s_{ij} \equiv 1$ and one near $s_{ij} \equiv -1$.)