Boltzmann pseudo-dynamics in glassy systems

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Overview

Overview of the presentation

- 1) Aging dynamics, the Spin Glass view
- 2) Ultra-Long time limit
- 3) Quasi-equilibrium picture
- 4) How glasses explore configuration space

Off-equilibrium relaxation in glassy systems

As we know from mean-field spin glasses.

$$\mathbf{S} = \{S_1, ..., S_N\}$$

Ising or spherical, interacting through a complicated Hamiltonian

$$H[\mathbf{S}]$$

Relaxational dynamics: sudden quench from a random high temperature initial condition $\mathbf{S}_0$.
large time dynamics, but $N \to \infty$ first.

Quantities of interest

- $E(t) = \langle H[S_t] \rangle$, $m(t) = \frac{1}{N} \sum_i \langle S_i(t) \rangle$
- $C(t, t_w) = \frac{1}{N} \sum_i \langle S_i(t) S_i(t_w) \rangle$
- Linear response function to a field acting from t_w to t: $\chi(t, t_w) = \int_{t_w}^{t} du \, R(t, u)$

Prejudism: Any

- local dynamics
- respecting detailed balance

gives the same long time behaviour.

Aging at low temperature

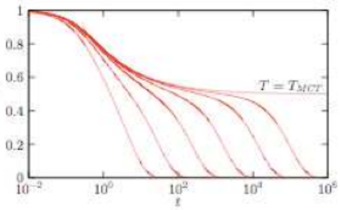
For large t:

$E(t) \to E_\infty$, $m(t) \to m_\infty$ (typically as powers of t) t, t_w large

$$\lim_{\substack{t,t_w \to \infty \\ t-t_w=\tau}} C(t,t_w) = C_{st}(\tau)$$

Other non-trivial relaxation regimes where C relaxes below the value of $q = \lim_{\tau\to\infty} C_{st}(\tau)$. In the simplest case (1RSB) $\tau_{rel}(t_w) \to \infty$ for $t_w \to \infty$

$$\lim_{\substack{t,t_w \to \infty \\ t-t_w=\tau_{rel}(t_w)}} C(t,t_w) = C_{st}(\tau)$$



Important characterization:

$$X(c) = \lim_{\substack{t,t_w\to\infty \\ C(t,t_w)=c}} -T\frac{R(t,t_w)}{\partial C(t,t_w)/\partial t_w}$$

1RSB systems $X(c) = X = const. < 1$ for $c < q$
FRSB systems $X(c)$ continuous monotonous function in $[0, q]$

$T/X(c)$ effective temperature. Degrees of freedom evolving on the same time scale are in mutual equilibrium (Cugliandono, Kurchan, Peliti '97).

Questions:

- **Can we understand the way in which glassy systems sample the space of configurations ?**
- **Can we find approximation schemes to study long time dynamics in realistic models ?**

Relation with equilibrium: Ultra long time limit

$X(c)$ can be related to Parisi's equilibrium function $P(q)$ for *Stochastically stable* systems.
Perturb the Hamiltonian with terms of the kind $\epsilon H_p(S)$ where $E(H_p(S)H_p(S')) = N\, q(S,S')^p$. Then in equilibrium

$$\langle H_p(S) \rangle_{eq} = \epsilon\beta[1 - \int_0^1 dq\; P(q)\; q^p$$

while in dynamics

$$\langle H_p(S_t) \rangle_{dyn} = \epsilon \int_0^t pC(t,u)^{p-1} R(t,u)\; du$$

If $\langle H_p(S_t) \rangle_{dyn} \to \langle H_p(S) \rangle_{eq}$ then $X(c) = \int_0^c P(q')\, dq'$
(SF, M. Mezard, G. Parisi, L. Peliti 1998).

1RSB behavior

Equilibration of 1 time quantities happens in SK, it is expected in finite D, but does not occur in the p-spin model.
Aging associated to clustering (rather than thermodynamic) transition
Threshold metastable states with free-energy f_{th}
$\Sigma(f, T)$ complexity

$$\beta X = \frac{\partial}{\partial f} \Sigma(f_{th}, T).$$

Important relation between dynamics and thermodynamics.
Rationalization: Quasi-equilibrium picture

- Fast relaxation into metastable state, followed by relaxation in a complex landscape at much longer times
- Long time dynamics proceeds as a random walk between metastable state, where *dynamically available states* at a given time are sampled with Boltzmann probability.

(SF, M. Virasoro 2000)

Formalization: Boltzmann pseudo-dnamics

Coarse grain short time: collapse the time needed to go to $q_{EA} - \epsilon$
Markov chain:

$$M(S_{\tau+1}|S_\tau) = \frac{1}{Z[S_\tau]} \exp(-\beta H(S_{\tau+1}))\delta(q(S_{\tau+1}, S_\tau) - q)$$

or

$$\tilde{M}(S_{\tau+1}|S_\tau) = \frac{1}{Z[S_\tau]} \exp(-\beta H(S_{\tau+1}) - N\nu_\tau q(S_{\tau+1}, S_\tau))$$

Response function

Dynamics in a time dependent field h_τ coupled with an observable $m(\mathbf{S}_\tau)$,

$$H_h(\mathbf{S}_\tau, \tau) = H(\mathbf{S}_\tau) - h_\tau m(\mathbf{S}_\tau).$$
$$\Delta(\tau, \sigma)) = \frac{\partial \langle m(\mathbf{S}_\tau) \rangle}{\partial h_\sigma}$$

To compute this quantity we just need

$$\frac{\partial}{\partial h_s} P\left(\mathbf{S}_1^\tau | \mathbf{S}_0\right) =$$
$$\beta \left[m(\mathbf{S}_\sigma) - E\left[m | \mathbf{S}_{j-1} \right] \right] P\left(\mathbf{S}_1^\tau | \mathbf{S}_0\right)$$

$$E\left[m|\mathbf{S}_{\sigma-1}\right] = \frac{1}{Z[\mathbf{S}_{\sigma-1}]} \sum_S e^{-\beta H(\mathbf{S})} m(\underline{S}) \delta\left(q(\mathbf{S}, \mathbf{S}_{\sigma-1}) - \tilde{q}\right).$$

$$R(\tau, \sigma) = \beta[\langle m(\mathbf{S}_\tau) m(\mathbf{S}_\sigma) \rangle - \langle m_\tau E(m|\mathbf{S}_{\sigma-1}) \rangle] = \beta[C(\tau, \sigma) - D(\tau, \sigma)]$$

Spherical spin glasses

Closed Dynamic Equations for $C(\tau,\sigma)$ and $R(\tau,\sigma)$:
$J_{i,j,k} = \mathcal{N}(0, 1/N^2)$

$$H[S] = \sum_{i<j<k}^{1,N} J_{ijk} S_i S_j S_k$$

Consider a function, or operator $f(\mathbf{S})$:

$$E_J \int d\mu(\mathbf{S}_1^\tau)\, \frac{\partial}{\partial S_j(\sigma)} f(\mathbf{S}_1^\tau) P(\mathbf{S}_1^\tau | \{\mathbf{S}_0\}) = 0$$

- Choose $f(\mathbf{S}) = S_i(j)$ and $f(\mathbf{S}) = \frac{\partial}{\partial h}$
- Integrate by parts over the J_{ijk}
- Assume $i \neq j$,
  $\langle S_i(\tau) S_i(\sigma) S_j(\tau) S_j(\sigma)\rangle \approx \langle S_i(\tau) S_i(\sigma)\rangle \langle S_j(\tau) S_j(\sigma)\rangle$

Closed coupled integral equations for $C(\tau,\sigma)$ and $D(\tau,\sigma)$.
"Long chain limit" L chain length $\to\infty$, t/τ continuous.
$\Delta(t,u) = D(t,u) - C(t,u) = TR(t,u)du$

$$
\begin{aligned}
0 &= \beta\int_0^t du\, 3C^2(s,u)R(t,u) + \beta\int_0^s du\, 6C(s,u)R(s,u)C(t,u) \\
&\quad +3\beta^2(1-q^2)C(t,u) + 3\beta^2 C(t,u)^2(1-q) - \mu C(t,s) - \nu C(t,s) \\
0 &= \beta\int_s^t du\, 6R(t,u)C(u,s)R(u,s) + 6\beta C(t,u)R(t,u)(1-q) + \\
&\quad 3\beta q^2 R(t,u) - \mu R(t,s) - \nu R(t,s)
\end{aligned}
$$

μ spherical constraint
ν chain constraint
Consistency if $\nu_s \to 0$: Aging (time reparametrization invariant) part of the Cugliandolo-Kurchan equations for the p-spin model with Langevin dynamics.

Replicas

Get rid of annoying denominator in $M(S|S') = \frac{1}{Z[S']} e^{-\beta H} \delta(...)$

$$M_{n_\tau}(S_{\tau+1}|S_\tau) = Z[S_\tau]^{n_\tau - 1} \exp(-\beta H(S_{\tau+1}))\delta(q(S_{\tau+1}, S_\tau) - q_{EA})$$

$$= \sum_{S_\tau^a;(a=1,...,n_\tau-1)} \exp(-\beta \sum_{a=0}^{n_\tau} H(S_{\tau+1}^a)) \prod_{a=0}^{n_\tau-1} \delta(q(S_{\tau+1}^a, S_\tau^a) - q_{EA})$$

$S^0 \equiv S$ master;
$S^a \quad a = 1, ..., n_\tau - 1$ slaves.
$n_\tau \to 0$ at the end of the computations.

Replicas II

- Advantage: formalism close to equilibrium.
- $P_n(\mathbf{S}_1^\tau|\mathbf{S}_0)$ has the form of a Boltzmann probability
- Alternative derivation of equations in spherical models.
- Replica order parameter $Q_{a,b}(t,s)$
- RS ansatz

$$
\begin{aligned}
Q_{a,b}(t,s) &= C(t,s) + TR(t,s)ds\delta_{b,0} + TR(s,t)dt\delta_{a,0} \\
&\quad +(1-q)\delta(t-s)\delta_{a,b}
\end{aligned}
$$

- In theory of liquids, models are not exactly solvable.
- Any approximation available for equilibrium can be used to study long time dynamics (e.g. HNC).

Conclusions

- Formalization of notion of quasi-equilibrium sampling of configuration spaces in glassy systems
- It reproduce the results of bona-fide relaxational dynamics in Mean-Field
- Same results with and without replicas
- Formal analogy with Boltzmann measure in the replica
- Use equilibrium approximation schemes in realistic systems to study glassy long time dynamics.