Open nonequilibrium problems in spin systems

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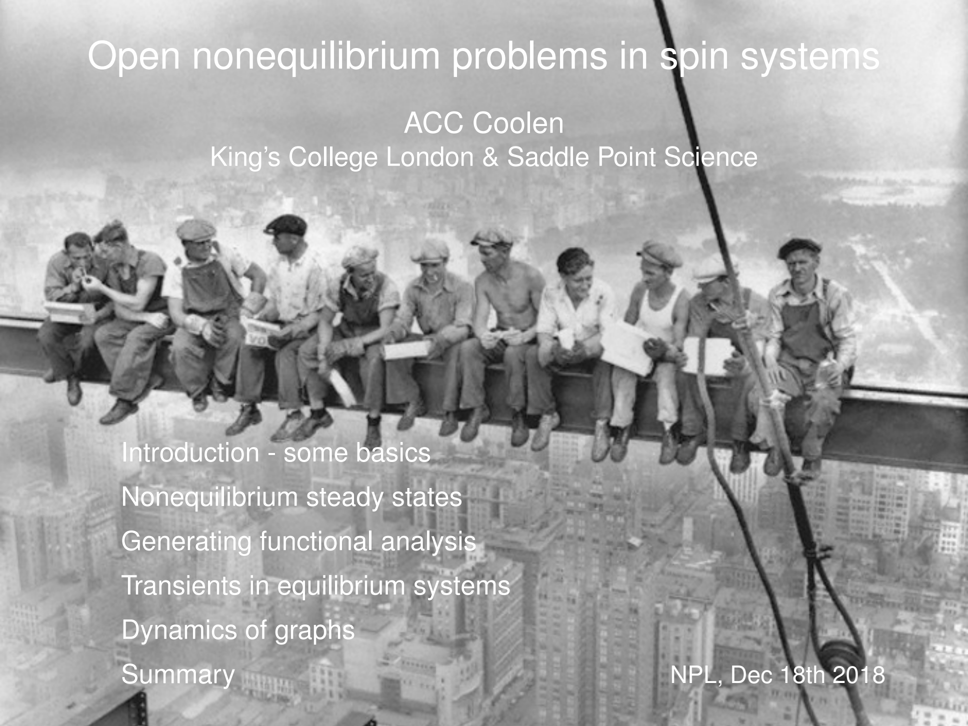

Introduction - some basics

Nonequilibrium steady states

Generating functional analysis

Transients in equilibrium systems

Dynamics of graphs

Summary

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Stochastic dynamical spin systems

$\boldsymbol{\sigma}(t) = (\sigma_1(t), \ldots, \sigma_N(t))$

Ising variables, discrete time:

- Markovian dynamics:

$$parallel: \quad \sigma_i(t+1) = sgn[h_i(\boldsymbol{\sigma}(t)) + T\eta_i(t)] \quad \forall i$$

$$sequential: \quad \sigma_i(t+1) = sgn[h_i(\boldsymbol{\sigma}(t)) + T\eta_i(t)] \quad if \;\; i = i_t$$

$$\sigma_i(t+1) = \sigma_i(t) \quad if \;\; i \neq i_t$$

i_t : *drawn indep from* $\{1, \ldots, N\}$

- local fields:

$$h_i(\boldsymbol{\sigma}) = \theta_i + \sum_j J_{ij}\sigma_j + \sum_{jk} J_{ijk}\sigma_j\sigma_k + \ldots$$

- noise $\eta_i(t) \in \mathbb{R}$:

  drawn indep from $p(\eta)$,
  with $p(-\eta) = p(\eta)$

generalizations:

random index sets $S \subseteq \{1, \ldots, N\}$
updated at each step,
Potts spins $\sigma_i \in \{1, \ldots, q\}$,
etc

Continuous variables, continuous time:

- Langevin dynamics: $$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_i(t) = f_i(\boldsymbol{\sigma}(t)) + \eta_i(t) \qquad \forall i$$
- forces: $$f_i(\boldsymbol{\sigma}) = \theta_i + \sum_j J_{ij}\sigma_j + \sum_{jk} J_{ijk}\sigma_j\sigma_k + \ldots$$
- Gaussian noise $\eta_i(t) \in \mathbb{R}$:

  $\langle \eta_i(t) \rangle = 0, \ \langle \eta_i(t)\eta_j(t') \rangle = 2T\delta_{ij}\delta(t-t')$

defined as limit $\Delta \downarrow 0$ of

$$\sigma_i(t+\Delta) = \sigma_i(t) + \Delta f_i(\boldsymbol{\sigma}(t)) + \sqrt{2T\Delta}\,\xi_i(t)$$

$\eta_i(t) = \xi_i(t)\sqrt{2T/\Delta}$ — *Itô* : $\xi_i(t)$ *indep Gaussian*

Stratonovich : $\xi_i(t)$ *correl Gaussian*

generalizations:

non-Gaussian noise,
spherical spins, $\boldsymbol{\sigma}^2(t) = N$,
etc

Description in term of state probabilities

- Ising spins, parallel dynamics:

$$\sigma_i(t+1) = sgn[h_i(\boldsymbol{\sigma}(t)) + T\eta_i(t)] \qquad \forall i$$

$$\Leftrightarrow$$

$$p_{t+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p_t(\boldsymbol{\sigma}'), \qquad W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] = \prod_i \frac{1}{2}[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}'))]$$

$$\beta = 1/T, \quad g(x) = 2\int_{-\infty}^{x} \mathrm{d}\eta\, p(\eta)$$

- Ising spins, sequential dynamics:

$$\sigma_i(\ell+1) = \delta_{i,i_\ell}\, sgn[h_i(\boldsymbol{\sigma}(\ell)) + T\eta_i(\ell)] + (1-\delta_{i,i_\ell})\sigma_i(\ell)$$

$$\textit{random step durations}: \quad \mathrm{prob}(\ell|t) = (t/\Delta)^\ell \mathrm{e}^{-t/\Delta}/\ell!, \qquad \Delta = N^{-1}$$

$$\Leftrightarrow$$

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = \sum_i \Big[w_i(F_i\boldsymbol{\sigma})p_t(F_i\boldsymbol{\sigma}) - w_i(\boldsymbol{\sigma})p_t(\boldsymbol{\sigma})\Big] \quad (\textit{master eqn})$$

$$F_i\boldsymbol{\sigma} = (\sigma_1,\ldots,-\sigma_i,\ldots,\sigma_N), \qquad w_i(\boldsymbol{\sigma}) = \frac{1}{2}[1-\sigma_i g(\beta h_i(\boldsymbol{\sigma}))]$$

- continuous spins, Langevin dynamics:

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_i(t) = f_i(\boldsymbol{\sigma}(t)) + \eta_i(t) \qquad \forall i$$

$$\Leftrightarrow$$

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = -\sum_i \frac{\partial}{\partial \sigma_i}\left[f_i(\boldsymbol{\sigma})p_t(\boldsymbol{\sigma}) - T\frac{\partial}{\partial \sigma_i}p_t(\boldsymbol{\sigma})\right] \quad (\textit{Fokker}-\textit{Planck eqn})$$

common form

linear eqns for $p_t = \{p_t(\boldsymbol{\sigma})\}$

$$p_{t+1} = Wp_t, \quad \frac{\mathrm{d}}{\mathrm{d}t}p_t = (W - 1\!\!1)p_t$$

common questions

- existence & uniqueness of stationary states: $Wp_\infty = p_\infty$
- formula for stationary states p_∞
- transients, evolution towards p_∞

Equilibrium states

special stationary solutions $p(\boldsymbol{\sigma})$
that obey *detailed balance*:

$$(\forall \boldsymbol{\sigma}, \boldsymbol{\sigma}') : \qquad \mathrm{Prob}\big[\textit{observing } \boldsymbol{\sigma} \to \boldsymbol{\sigma}'\big] = \mathrm{Prob}\big[\textit{observing } \boldsymbol{\sigma}' \to \boldsymbol{\sigma}\big]$$

for instance:

$$p_{t+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}; \boldsymbol{\sigma}'] p_t(\boldsymbol{\sigma}') : \qquad W[\boldsymbol{\sigma}; \boldsymbol{\sigma}'] p(\boldsymbol{\sigma}') = W[\boldsymbol{\sigma}'; \boldsymbol{\sigma}] p(\boldsymbol{\sigma})$$

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(\boldsymbol{\sigma}) = \sum_i \Big[w_i(F_i\boldsymbol{\sigma}) p_t(F_i\boldsymbol{\sigma}) - w_i(\boldsymbol{\sigma}) p_t(\boldsymbol{\sigma}) \Big] : \qquad w_i(F_i\boldsymbol{\sigma}) p(F_i\boldsymbol{\sigma}) = w_i(\boldsymbol{\sigma}) p(\boldsymbol{\sigma})$$

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(\boldsymbol{\sigma}) = -\sum_i \frac{\partial}{\partial \sigma_i} \Big[f_i(\boldsymbol{\sigma}) p_t(\boldsymbol{\sigma}) - T \frac{\partial}{\partial \sigma_i} p_t(\boldsymbol{\sigma}) \Big] : \qquad f_i(\boldsymbol{\sigma}) p(\boldsymbol{\sigma}) = T \frac{\partial}{\partial \sigma_i} p(\boldsymbol{\sigma})$$

many benefits!

– route for *finding* $p(\boldsymbol{\sigma})$, leads to equil stat mech
– prove uniqueness of $p(\boldsymbol{\sigma})$, and convergence
– FDT relations
– MCMC sampling *but requires special properties of forces and noise!*

detailed balance – tool for finding $p(\boldsymbol{\sigma})$

if we choose

$h_i(\boldsymbol{\sigma}) = \sum_j J_{ij}\sigma_j + \theta_i, \quad J_{ij} = J_{ji}$

$p(\eta) = \frac{1}{2}[1 - \tanh^2(\eta)]$, so $g(h) = \tanh(h)$

- Ising spins, sequential dyn (master eqn):

  $w_i(F_i\boldsymbol{\sigma})p(F_i\boldsymbol{\sigma}) = w_i(\boldsymbol{\sigma})p(\boldsymbol{\sigma}), \; J_{ii} = 0:$ $\quad p(\boldsymbol{\sigma}) \propto \mathrm{e}^{\beta\left[\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j + \sum_i \theta_i\sigma_i\right]}$

- Ising spins, parallel dyn:

  $W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p(\boldsymbol{\sigma}') = W[\boldsymbol{\sigma}';\boldsymbol{\sigma}]p(\boldsymbol{\sigma}):$

  $$p(\boldsymbol{\sigma}) \propto \mathrm{e}^{\beta\sum_i \theta_i\sigma_i} \prod_i \cosh[\beta(\theta_i + \sum_j J_{ij}\sigma_j)] = \sum_{\boldsymbol{\sigma}'} \mathrm{e}^{\beta\left[\sum_{ij} J_{ij}\sigma_i'\sigma_j + \sum_i \theta_i(\sigma_i' + \sigma_i)\right]}$$

- continuous spins:
  (Fokker-Planck eqn)

  $$f_i(\boldsymbol{\sigma}) = T\frac{\partial}{\partial\sigma_i}\log p(\boldsymbol{\sigma}),$$
  $$f_i(\boldsymbol{\sigma}) = h_i(\boldsymbol{\sigma}) + \frac{\partial}{\partial\sigma_i}V(\sigma_i):$$

  $$p(\boldsymbol{\sigma}) \propto \mathrm{e}^{\beta\left[\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j + \sum_i \theta_i\sigma_i - \sum_i V(\sigma_i)\right]}$$

detailed balance – uniqueness and convergence, the H-theorem

$p_\infty(\boldsymbol{\sigma}) = Z^{-1}\exp[-\beta H(\boldsymbol{\sigma})]$:

$$\mathcal{H}(t) = \frac{1}{\beta} D(p_t||p_\infty) \;=\; \begin{cases} \beta^{-1}\sum_{\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma}) \log\left[p_t(\boldsymbol{\sigma})/p_\infty(\boldsymbol{\sigma})\right] & (\textit{Ising}) \\ \beta^{-1}\int \mathrm{d}\boldsymbol{\sigma}\; p_t(\boldsymbol{\sigma}) \log\left[p_t(\boldsymbol{\sigma})/p_\infty(\boldsymbol{\sigma})\right] & (\textit{continuous}) \end{cases}$$

$$= \begin{cases} \sum_{\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma})\left[H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma})\right] + \frac{1}{\beta}\log Z & (\textit{Ising}) \\ \int \mathrm{d}\boldsymbol{\sigma}\; p_t(\boldsymbol{\sigma})\left[H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma})\right] + \frac{1}{\beta}\log Z & (\textit{cont}) \end{cases}$$

$$= \quad E(t) - TS(t) + \beta^{-1}\log Z \quad (\textit{dynamic free energy})$$

if process ergodic:

- Ising spins: master eqn — $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(t) \leq 0$, *stationary iff* $p = p_\infty$
- continuous spins: Fokker-Planck eqn — $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(t) \leq 0$, *stationary iff* $p = p_\infty$
- Ising spins: parallel dynamics — $\mathcal{H}(t+1) - \mathcal{H}(t) = ?$, *not yet done, probably easy...*

detailed balance essential in proofs!

detailed balance – fluctuation dissipation theorems (FDT)

let $\theta_i \to \theta_i(t)$:

$$C_{ij}(t,t') = \langle \sigma_i(t)\sigma_j(t')\rangle, \qquad G_{ij}(t,t') = \partial\langle\sigma_i(t)\rangle/\partial\theta_j(t')$$

derivation:

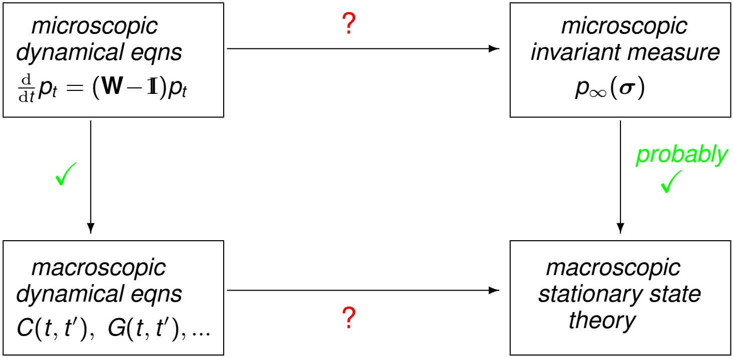
(i) differentiate stat state eqn wrt external fields
(ii) use $C_{ij}(t,t') = C_{ij}(t-t')$ and $G_{ij}(t,t') = G_{ij}(t-t')$
(iii) use detailed balance condition to simplify

- Ising spins, master eqn: $$G_{ij}(\tau) = -\beta\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}C_{ij}(\tau)$$
- continuous spins, Fokker-Planck eqn: $$G_{ij}(\tau) = -\beta\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}C_{ij}(\tau)$$
- Ising spins, parallel dyn: $$G_{ij}(\tau>0) = -\beta\left[C_{ij}(\tau+1) - C_{ij}(\tau-1)\right]$$ $$G_{ij}(\tau\leq 0) = 0$$

generalizations to higher order FDTs
detailed balance essential in derivations!

access to
non-equilibrium
stationary state physics

most real world processes
(physics, biology, chemistry, economics)
do *not* obey detailed balance ...



Nonequilbrium steady states

most real world processes
do *not* obey detailed balance ...

yet many go to unique stationary state
(Perron-Frobenius theorem)
but $p(\boldsymbol{\sigma})$ tricky to compute ...

- Ising spins,
  parallel dyn: $$p(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p(\boldsymbol{\sigma}')$$
- Ising spins,
  master eqn: $$\sum_i \Big[w_i(F_i\boldsymbol{\sigma})p(F_i\boldsymbol{\sigma}) - w_i(\boldsymbol{\sigma})p(\boldsymbol{\sigma})\Big] = 0$$
- continuous spins,
  Langevin dyn: $$\sum_i \frac{\partial}{\partial\sigma_i}\Big[f_i(\boldsymbol{\sigma})p(\boldsymbol{\sigma}) - T\frac{\partial}{\partial\sigma_i}p(\boldsymbol{\sigma})\Big] = 0$$

detailed balance violations

– noise induced, i.e. $p(\eta) \neq \frac{1}{2}[1-\tanh^2(\eta)]$

– force induced, e.g. $J_{ij} \neq J_{ji}$ ...

noise induced violation of detailed balance

e.g. master eqn, Ising spins

$h_i(\boldsymbol{\sigma}) = \sum_j J_{ij}\sigma_j + \theta_i,$

$J_{ij} = J_{ji}, \;\; J_{ii} = 0$

$$\begin{aligned} p(\eta) &= \tfrac{1}{2}[1-\tanh^2(\eta)] \\ g(x) &= \tanh(x) \end{aligned} \quad \rightarrow \quad \begin{aligned} p(\eta) &= \mathrm{e}^{-\frac{1}{2}\eta^2}/\sqrt{2\pi} \\ g(x) &= \mathrm{Erf}(x/\sqrt{2}) \end{aligned}$$

stationary state eqn:

$$\sum_i \left[p(F_i\boldsymbol{\sigma})\mathrm{e}^{\sigma_i \tanh^{-1}\left[\mathrm{Erf}\left(\frac{\beta}{\sqrt{2}}(\theta_i+\sum_j J_{ij}\sigma_j)\right)\right]} - p(\boldsymbol{\sigma})\mathrm{e}^{-\sigma_i \tanh^{-1}\left[\mathrm{Erf}\left(\frac{\beta}{\sqrt{2}}(\theta_i+\sum_j J_{ij}\sigma_j)\right)\right]} \right] = 0$$

questions

- intuition:

  'internal' forces still as in conventional defns,
  Gaussian noise natural (CLT?) for representing environment,
  why does a heat bath require $p(\eta) = \frac{1}{2}[1-\tanh^2(\eta)]$?
- mathematical: what is $p(\boldsymbol{\sigma})$?

force induced violation of detailed balance

- e.g. Fokker-Planck eqn, continuous spins, special case:

$$p(\boldsymbol{\sigma}) = \mathrm{e}^{-\beta H(\boldsymbol{\sigma})},$$

$$f_i(\boldsymbol{\sigma}) = -\frac{\partial}{\partial \sigma_i} H(\boldsymbol{\sigma}) + F_i(\boldsymbol{\sigma})\mathrm{e}^{\beta H(\boldsymbol{\sigma})}$$

  stationary state:

$$\sum_i \frac{\partial F_i(\boldsymbol{\sigma})}{\partial \sigma_i} = 0$$

- e.g. master eqn, Ising spins

$$p(\eta) = \tfrac{1}{2}[1-\tanh^2(\eta)],$$

$$h_i(\boldsymbol{\sigma}) = \textstyle\sum_j J_{ij}\sigma_j + \theta_i, \;\; J_{ii} = 0 \qquad J_{ij} = J_{ij}^+ + J_{ij}^-, \quad \begin{cases} J_{ji}^+ = J_{ij}^+ \\ J_{ji}^- = -J_{ij}^- \end{cases}$$

  stationary state:

$$p(\boldsymbol{\sigma}) = q(\boldsymbol{\sigma})\mathrm{e}^{\beta \sum_j \theta_j \sigma_j + \frac{1}{2}\beta \sum_{ij} J_{ij}^+ \sigma_i \sigma_j} : \qquad q(\boldsymbol{\sigma}) = \frac{\sum_i \mathrm{e}^{\beta \sigma_i \sum_j J_{ij}^- \sigma_j} q(F_i \boldsymbol{\sigma})}{\sum_i \mathrm{e}^{-\beta \sigma_i \sum_j J_{ij}^- \sigma_j}}$$

  question: what is $q(\boldsymbol{\sigma})$?
  only first few orders in β expansion known ...

Generating functional analysis

derivation of macroscopic dynamical eqns
for heterogeneous systems

- generating functional: average over all paths $\{\boldsymbol{\sigma}(t)\}$
  (if $t\in\mathbb{R}$: $\sum_t\to\int\mathrm{d}t$)

$$
\begin{aligned}
Z[\boldsymbol{\psi}] &= \left\langle \mathrm{e}^{-\mathrm{i}\sum_i\sum_t \psi_i(t)\sigma_i(t)} \right\rangle \\
&= \sum_{\{\boldsymbol{\sigma}\}} \mathrm{e}^{-\mathrm{i}\sum_i\sum_t \psi_i(t)\sigma_i(t)} p(\{\boldsymbol{\sigma}\}) \\
&= \sum_{\{\boldsymbol{\sigma}\}} \mathrm{e}^{-\mathrm{i}\sum_i\sum_t \psi_i(t)\sigma_i(t)} p_0(\boldsymbol{\sigma}(0)) \prod_{t\geq 0} W_t[\boldsymbol{\sigma}(t+1);\boldsymbol{\sigma}(t)]
\end{aligned}
$$

now

$$
\langle\sigma_i(t)\rangle = \mathrm{i}\lim_{\boldsymbol{\psi}\to 0}\frac{\partial Z[\boldsymbol{\psi}]}{\partial\psi_i(t)}, \qquad \frac{\partial\langle\sigma_i(t)\rangle}{\partial\theta_j(t')} = \mathrm{i}\lim_{\boldsymbol{\psi}\to 0}\frac{\partial^2 Z[\boldsymbol{\psi}]}{\partial\psi_i(t)\partial\theta_j(t')},
$$

$$
\langle\sigma_i(t)\sigma_j(t')\rangle = -\lim_{\boldsymbol{\psi}\to 0}\frac{\partial^2 Z[\boldsymbol{\psi}]}{\partial\psi_i(t)\partial\psi_j(t')} \qquad \textit{etc}
$$

disorder: $\{J_{ij}\}$

- average over disorder

$$\overline{Z[\psi]} = \overline{\left\langle \mathrm{e}^{-\mathrm{i}\sum_i \sum_t \psi_i(t)\sigma_i(t)} \right\rangle} :$$

$$\overline{\langle \sigma_i(t) \rangle} = \lim_{\psi \to 0} \frac{\mathrm{i}\partial \overline{Z[\psi]}}{\partial \psi_i(t)}$$

$$C_{ij}(t,t') = -\lim_{\psi \to 0} \frac{\partial^2 \overline{Z[\psi]}}{\partial \psi_i(t) \partial \psi_j(t')}$$

$$G_{ij}(t,t') = \lim_{\psi \to 0} \frac{\mathrm{i}\partial^2 \overline{Z[\psi]}}{\partial \psi_i(t) \partial \theta_j(t')}$$

- computing $\overline{Z[\psi]}$

insert integral over field paths: $\{\mathbf{h}(t)\}$

$$1 = \int \prod_t \mathrm{d}\mathbf{h}(t) \prod_{ti} \delta\left[h_i(t) - \sum_j J_{ij}\sigma_j(t) - \theta_i(t)\right]$$

$$= \int \prod_t \frac{\mathrm{d}\mathbf{h}(t)\mathrm{d}\hat{\mathbf{h}}(t)}{(2\pi)^N} \prod_{ti} \mathrm{e}^{\mathrm{i}\hat{h}_i(t)\left[h_i(t) - \sum_j J_{ij}\sigma_j(t) - \theta_i(t)\right]}$$

so that

$$\overline{Z[\psi]} = \sum_{\{\sigma\}} p_0(\sigma(0)) \int \prod_t \left[\frac{\mathrm{d}\mathbf{h}(t)\mathrm{d}\hat{\mathbf{h}}(t)}{(2\pi)^N} \mathrm{e}^{\mathrm{i}\hat{\mathbf{h}}(t)\cdot\mathbf{h}(t) - \mathrm{i}\psi(t)\cdot\sigma(t)} \prod_i \frac{\mathrm{e}^{\beta\sigma_i(t+1)h_i(t)}}{2\cosh[\beta h_i(t)]} \right]$$

$$\times \overline{\mathrm{e}^{-\mathrm{i}\sum_{ij} J_{ij} \sum_t \hat{h}_i(t)\sigma_j(t)}}$$

← *easy! no need for DB...*

impact of connectivity scaling ...

early results

- fully connected, e.g.

SK type:

$$i<j: \quad p(J_{ij}) = \left(\frac{KN}{2\pi}\right)^{\frac{1}{2}} \mathrm{e}^{-\frac{1}{2}KNJ_{ij}^2}$$

$$i>j: \quad p(J_{ij}) = \eta \left(\frac{KN}{2\pi}\right)^{\frac{1}{2}} \mathrm{e}^{-\frac{1}{2}KNJ_{ij}^2} + (1-\eta)\delta(J_{ij}-J_{ji})$$

Hopfield type:

$$J_{ij} = \frac{1}{N}\sum_{\mu=1}^{\alpha N} \xi_i^\mu \xi_j^\mu \quad \textit{or} \quad J_{ij} = \frac{1}{N}\sum_{\mu=1}^{\alpha N} \xi_i^{\mu+1} \xi_j^\mu$$

- extremely diluted, e.g.

DGZ type:

$$J_{ij} = \frac{c_{ij}}{c}\sum_{\mu=1}^{\alpha N} \xi_i^\mu \xi_j^\mu, \quad p(c_{ij}) = \frac{c}{N}\delta_{c_{ij},1} + (1-\frac{c}{N})\delta_{c_{ij},0}, \quad \frac{c}{N}, \frac{1}{c} \to 0$$

all cases: closed theory for $C(t,t')$ and $G(t,t')$,
defined in terms of effective single spin eqn
with non-white noise and (possibly) retarded self-interaction

stationary state, doable iff:

(i) fully asymmetric bonds (no retarded self-interaction), easy ...
(ii) fully symmetric bonds (use FDT), hard ...

impact of connectivity scaling ...

more recent results

- finitely connected, i.e. $c = \mathcal{O}(1)$:

$$J_{ij} = Jc_{ij}, \qquad p(\mathbf{c}) \propto \Big(\prod_{i<j} \hat{p}(c_{ij}, c_{ji})\Big)\Big(\prod_i \delta_{k_i,\sum_j c_{ij}}\Big)$$

$$\hat{p}(c_{ij}) = w(c_{ij}), \quad \hat{p}(c_{ji}|c_{ij}) = \epsilon\delta_{c_{ij},c_{ji}} + (1-\epsilon)w(c_{ji})$$

$$w(c_{ij}) = \frac{c}{N}\delta_{c_{ij},1} + (1-\frac{c}{N})\delta_{c_{ij},0}$$

more complex order pars, again defined in terms of effective eqn for single spin $\boldsymbol{\sigma} = \{\sigma(t)\}$

$$P(\boldsymbol{\sigma}|\boldsymbol{\theta}) = \lim_{N\to\infty} \frac{1}{N}\overline{\langle\delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}_i}\rangle}\Big|_{\boldsymbol{\theta}_i\to\boldsymbol{\theta}_i+\boldsymbol{\theta}}$$

$$Q(\boldsymbol{\sigma}|\boldsymbol{\theta}) = \lim_{N\to\infty} \frac{1}{N}\overline{\langle\delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}_i}\rangle}\Big|_{\boldsymbol{\theta}_i\to\boldsymbol{\theta}_i+\boldsymbol{\theta},\ k_i\to k_i-1}$$

stationary state, doable iff:

(i) fully asymmetric bonds, easy ...
(ii) fully symmetric bonds, only leading orders in c^{-1}, hard ...

simplest case we cannot (yet) do:

$p(k) = \delta_{k,2}$,
$\epsilon = 1$ (detailed balance!),
initial time to $-\infty$:

$$\boldsymbol{\sigma} = \{\sigma(t)\} : \qquad Q(\boldsymbol{\sigma}|\boldsymbol{\sigma}') = \sum_{\boldsymbol{\sigma}''} Q(\boldsymbol{\sigma}''|\boldsymbol{\sigma}) \prod_t \frac{e^{\beta J \sigma(t+1)[\sigma'(t)+\sigma''(t)]}}{2\cosh[\beta J[\sigma'(t)+\sigma''(t)]]}$$

questions:

(i) what is the stationary order parameter?
(ii) eqn for stationary order parameter?

why can't we use equilibrium theory to guide us?
(not even a phase transition in this model ...)

– equilibrium (replica) theory: formulated in terms of *effective* fields
– dynamical (GFA) theory: formulated in terms of *real* fields ...

Transients in complex equilibrium systems

disordered periodic 1-dimensional spin chain

with parallel dynamics

$$h_i(\boldsymbol{\sigma}) = J_i\sigma_{i-1} + J_{i+1}\sigma_{i+1} + \theta_i, \quad W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] = \prod_i \frac{e^{\beta\sigma_i h_i(\boldsymbol{\sigma}')}}{2\cosh[\beta h_i(\boldsymbol{\sigma}')]}$$

- can use GFA, but model has spatial structure:
  no longer mean-field order pars $P(\boldsymbol{\sigma}|\boldsymbol{\theta})$, $Q(\boldsymbol{\sigma}|\boldsymbol{\theta})$

- dynamical version of transfer matrix:
  transfer *operator* $\langle \boldsymbol{\sigma}, \mathbf{h}, \hat{\mathbf{h}}|M|\boldsymbol{\sigma}', \mathbf{h}', \hat{\mathbf{h}}'\rangle$

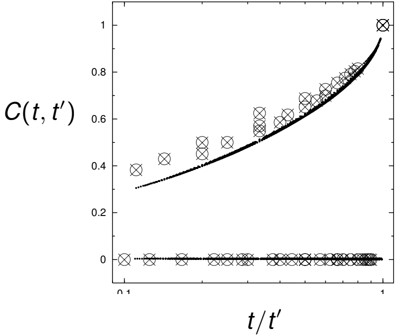
  acting on paths $\boldsymbol{\sigma} = \{\sigma(t)\}$, $\mathbf{h} = \{h(t)\}$, $\hat{\mathbf{h}} = \{\hat{h}(t)\}$

  largest eigenvalue: single-site dynamical observables
  (magnetizations, correlation- and response functions)

  second largest eigenvalue: correlation lengths e.g. anomalous relaxation in chains

$$p(\theta) = p(-\theta)$$
$$p(J) = \tfrac{1}{2}(1-\eta)\delta(J-\tilde{J}) + \tfrac{1}{2}(1+\eta)\delta(J+\tilde{J})$$

$$Q(\boldsymbol{\sigma}|\boldsymbol{\sigma}') = \sum_{\boldsymbol{\sigma}''} Q(\boldsymbol{\sigma}''|\boldsymbol{\sigma}') \int \mathrm{d}\theta\; p(\theta) \prod_t \frac{\mathrm{e}^{\beta\sigma(t+1)[\theta+\tilde{J}\sigma(t)+\tilde{J}\sigma''(t)]}}{\cosh[2\beta[\theta+\tilde{J}\sigma(t)+\tilde{J}\sigma''(t)]}$$
$$C(t,t') = \sum_{\boldsymbol{\sigma}} \sigma(t)\sigma(t') \sum_{\boldsymbol{\sigma}'} Q(\boldsymbol{\sigma}|\boldsymbol{\sigma}')Q(\boldsymbol{\sigma}'|\boldsymbol{\sigma}')$$



$\circ$ numerical soln of order par eqn

$\times$ simulations, $N = 10^6$

$t, t' = 1 \ldots 10$

$\cdot$ simulations, $50 \le t \le t' \le 100$

$T = 0.1$

analytical soln $Q(\boldsymbol{\sigma}|\boldsymbol{\sigma}')$?

Dynamics of graphs

constrained
Ising spin dynamics

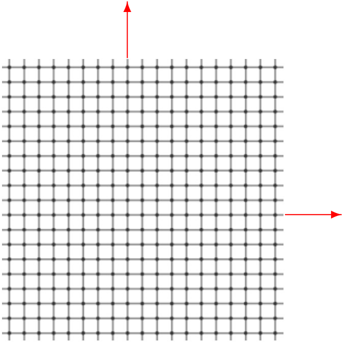
redefine

$N = n^2,\ \ \sigma_i = 2A_{k\ell} - 1,$
$M_s^{row} = 2k_s^{in} - n,$
$M_s^{col} = 2k_s^{out} - n,$

then

$A_{ij} \in \{0,1\},$
subject to
$\forall i:\ \sum_j A_{ij} = k_i^{in},$
$\forall i:\ \sum_j A_{ji} = k_i^{out}$

for all columns r:
$\sum_{i\ \text{in column}\ r} \sigma_i = M_r^{col}$



for all rows ℓ:
$\sum_{i\ \text{in row}\ s} \sigma_i = M_s^{row}$

stochastic evolution of *graphs* $\mathbf{A} = \{A_{ij}\}$,
with hard-constrained degrees

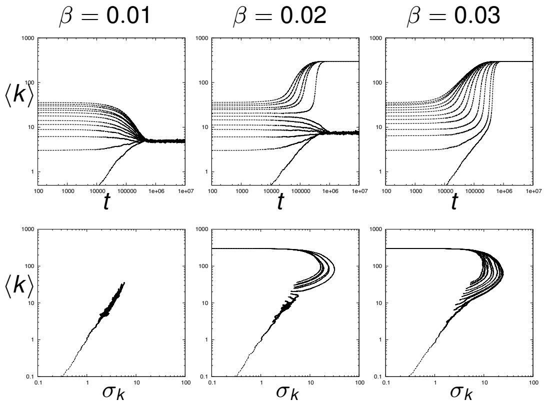
tricky new aspect: nr of possible moves not constant ...

why degree-constrained graph dynamics?

- generate soft-constrained nondirected graphs via MCMC

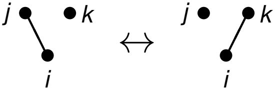
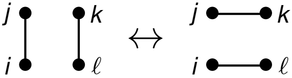
$$e.g. \quad p(\mathbf{A}) = \frac{1}{Z} \mathrm{e}^{\alpha \sum_i k_i(\mathbf{A}) + \beta \sum_i k_i^2(\mathbf{A})}$$

$$constrained: \quad \langle k \rangle = \frac{1}{N} \sum_i k_i(\mathbf{A}), \quad \langle k^2 \rangle = \frac{1}{N} \sum_i k_i^2(\mathbf{A})$$



$\alpha = 4, \quad N = 300$

MCMC for graphs with hard constraints

MOVE SET	INVARIANTS	ACTION
link flips $\{F_{ij}\}$	none	
hinge flips $\{F_{ijk}\}$	average degree $\bar{k}(\mathbf{A}) = \frac{1}{N}\sum_{rs} A_{rs}$	
edge swaps $\{F_{ijk\ell}\}$	all individual degrees $k_i(\mathbf{A}) = \sum_j A_{ij}$	

move acceptance probability
to achieve $p(\mathbf{A}) \propto \exp[-H(\mathbf{A})]$:

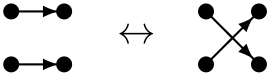
$$\mathcal{A}(\mathbf{A}|\mathbf{A}') = \frac{n(\mathbf{A}')\mathrm{e}^{-\frac{1}{2}[H(\mathbf{A})-H(\mathbf{A}')]}}{n(\mathbf{A}')\mathrm{e}^{-\frac{1}{2}[H(\mathbf{A})-H(\mathbf{A}')]} + n(\mathbf{A})\mathrm{e}^{\frac{1}{2}[H(\mathbf{A})-H(\mathbf{A}')]}}$$

$n(\mathbf{A})$: *nr of moves that can act on* $\mathbf{A}$

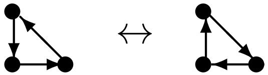
- edge swaps (conserve all degrees):

$$n(\mathbf{A}) = \underbrace{\frac{1}{4}N^2\langle k\rangle^2 + \frac{1}{4}N\langle k\rangle - \frac{1}{2}N\langle k^2\rangle}_{invariant} + \underbrace{\frac{1}{4}\mathrm{Tr}(\mathbf{A}^4) + \frac{1}{2}\mathrm{Tr}(\mathbf{A}^3) - \frac{1}{2}\sum_{ij} k_i A_{ij} k_j}_{state\ dependent}$$

- directed graphs, $A_{ij} \neq A_{ji}$,
  conserve all in- and out-degrees:



complication: edge swaps
not ergodic for directed graphs
further move type required:



$$n_{\square}(\mathbf{A}) = \underbrace{\frac{1}{2}N^2\langle k\rangle^2 - \sum_j k_j^{\mathrm{in}} k_j^{\mathrm{out}}}_{invariant} + \underbrace{\frac{1}{2}\mathrm{Tr}(\mathbf{A}^2) + \frac{1}{2}\mathrm{Tr}(\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger\mathbf{A}) + \mathrm{Tr}(\mathbf{A}^2\mathbf{A}^\dagger) - \sum_{ij} k_i^{\mathrm{in}} c_{ij} k_j^{\mathrm{out}}}_{state\ dependent}$$

$$n_{\triangle}(\mathbf{A}) = \underbrace{\frac{1}{3}\mathrm{Tr}(\mathbf{A}^3) - \mathrm{Tr}(\hat{\mathbf{A}}\mathbf{A}^2) + \mathrm{Tr}(\hat{\mathbf{A}}^2\mathbf{A}) - \frac{1}{3}\mathrm{Tr}(\hat{\mathbf{A}}^3)}_{state\ dependent}$$

with: $(\mathbf{A}^\dagger)_{ij} = A_{ji}$, $\hat{\mathbf{A}}_{ij} = A_{ij}A_{ji}$

picking candidate moves *randomly* ...

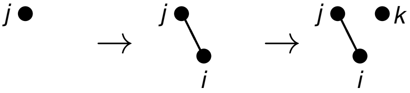
e.g. hinge flips

PROTOCOL 1:

(i) pick a site j with $k_j(\mathbf{A}) > 0$

(ii) pick a site $i \in \partial_j(\mathbf{A})$

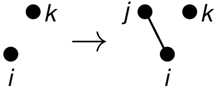
(iii) pick a site $k \notin \partial_i(\mathbf{A}) \cup \{i\}$



PROTOCOL 2:

(i) pick two disconnected sites (i, k) with $k_i(\mathbf{A}) > 0$

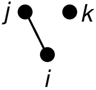
(ii) pick a site $j \in \partial_i(\mathbf{A})$



PROTOCOL 3:

(i) pick two connected sites (i, j) and a third site k

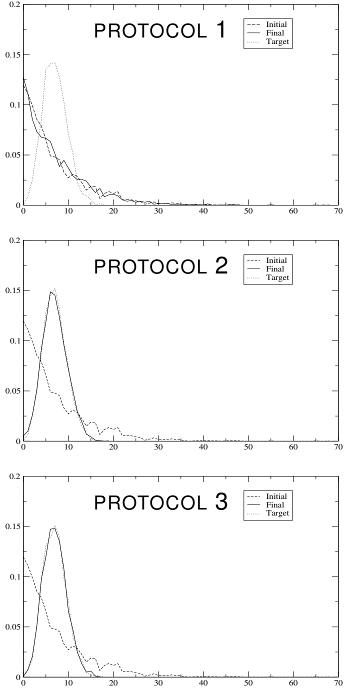
(ii) while $A_{ik} = 1$ return to (i)



$N = 3000$, $\langle k \rangle = 7$

initial graph: power law $p(k)$,
MCMC target: Poissonnian $p(k)$

dynamics highly sensitive
to correct move selection ...



Summary

- general, important and open
  (apart from special cases):

  computing microscopic invariant measure $p_\infty(\boldsymbol{\sigma})$
  for spin systems without detailed balance

- general, important and open
  (apart from special cases);

  extraction stationary state equations from GFA formalism
  for finitely connected random topologies
  (not even done yet for detailed balance ...)

- dynamics of 1-dim disordered systems:

  dynamical version of transfer matrix in GFA
  generalization to 2-dim?

- hard-constrained MCMC of graphs:

  interesting effects due to nr of possible moves not fixed
  (changing connection between dynamics and invariant measure)

papers, seminars, notes:
https://nms.kcl.ac.uk/ton.coolen