An observation concerning the effect of the Random Batch Method on phase transition

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I. Motivation

Simulation of particle systems

Consider a N particle system

$$dX_t^i = \frac{1}{N-1}\sum_{j\neq i} F(X_t^i - X_t^j)dt + \sqrt{2\sigma}dB_t^i, \tag{IPS}$$

which is linked to

$$\begin{cases} d\bar{X}_t = F * \bar{\rho}_t(\bar{X}_t)dt + \sqrt{2\sigma}dB_t, \\ \bar{\rho}_t = \text{Law}(\bar{X}_t). \end{cases} \tag{NL}$$

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Solution : Random Batch Method

Références :

Shi Jin, Lei Li, and Jian-Guo Liu. *Random batch methods (RBM) for interacting particles ystems.* J. Comput. Phys. (2020).

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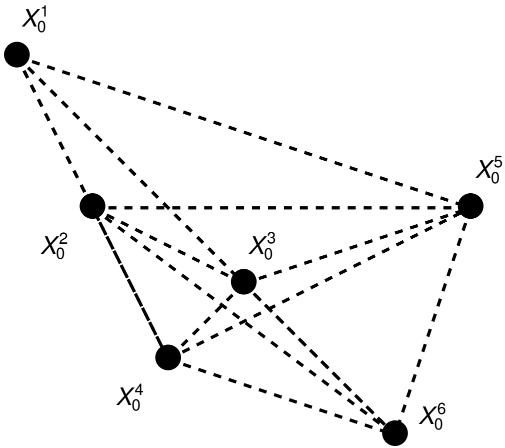

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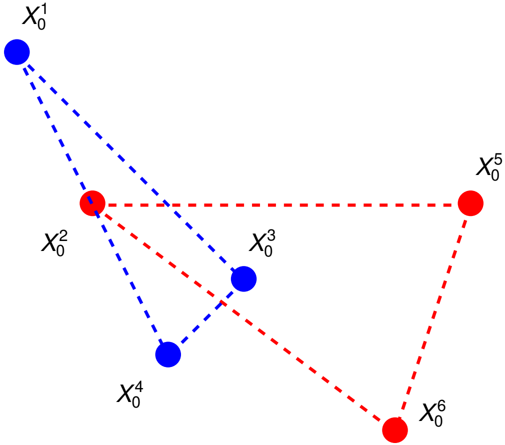

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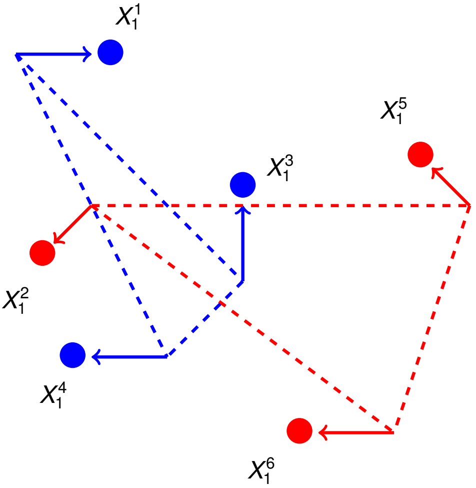

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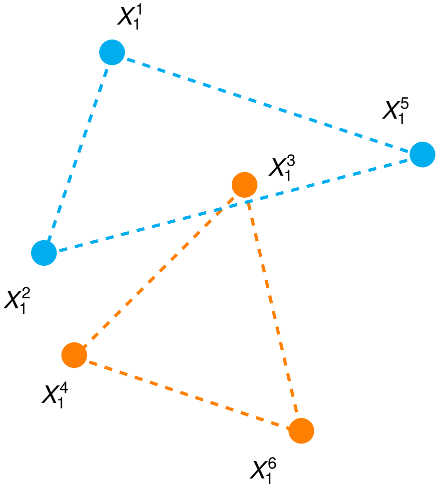

Addition of randomness

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Convergence as $N \to \infty$ with p fixed (Jin-Li '22)

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Writing

$$\xi_k = \frac{1}{p-1} \sum_{j=1}^{p-1} F\left(\bar{Y}_k^{\delta,p} - Y^j\right) \implies \mathbb{E}\left(\xi_t \middle| \bar{Y}_k^{\delta,p}\right) = F * \bar{\rho}_k^{\delta,p}(\bar{Y}_k^{\delta,p}),$$

$$\text{and} \quad \text{Var}\left(\xi_t \middle| \bar{Y}_t^{\delta,p}\right) = \frac{1}{p-1} \left(F^2 * \bar{\rho}_k^{\delta,p}(\bar{Y}_k^{\delta,p}) - (F * \bar{\rho}_k^{\delta,p}(\bar{Y}_k^{\delta,p}))^2\right).$$

Hence,

$$\bar{Y}_k^{\delta,p} = \bar{Y}_0^{\delta,p} + \delta \sum_{l=0}^{k-1} F * \bar{\rho}_l^{\delta,p}(\bar{Y}_l^{\delta,p}) - \delta M_k + \sqrt{2\sigma\delta} \sum_{l=0}^{k-1} G_l,$$

where $k \mapsto M_k := \sum_{l=0}^{k-1} \left(\xi_l - F * \bar{\rho}_l^{\delta,p}(\bar{Y}_l^{\delta,p})\right)$ is a martingale.

Effective dynamics

By martingale CLT, (D-RB-IPS) is close to the *effective dynamics*:

$$\begin{cases} d\bar{X}_t^{e,\delta,p} = F * \bar{\rho}_t^{e,\delta,p}(\bar{X}_t^{e,\delta,p})dt + \left(2\sigma + \frac{\delta}{p-1}\Sigma(\bar{X}_t^{e,\delta,p}, \bar{\rho}_t^{e,\delta,p})\right)^{1/2} dB_t, \\ \bar{\rho}_t^{e,\delta,p} = \mathrm{Law}(\bar{X}_t^{e,\delta,p}), \end{cases} \tag{Eff}$$

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Recall (NL)**:**

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Recall (D-RB-IPS)**:**

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How does this added randomness affects the nonlinear limit, and more precisely its phase transition ?

II. Understanding the problem on a toy model

II.1 The Curie-Weiss model

Markov chain

Let N spins $\sigma = (\sigma_1, ..., \sigma_N) \in \Omega_N = \{-1, 1\}^N$ and consider

$$\forall \sigma \in \Omega_N, \quad H_N(\sigma) = -\frac{1}{2N}\sum_{i,j} \sigma_i \sigma_j.$$

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- Accept $\sigma(k+1) = \sigma'$ with probability $e^{-\beta(H_N(\sigma') - H_N(\sigma(k)))_+}$ where β is the inverse temperature.

Mean magnetization

The system is entirely defined by its mean magnetization $m_N(\sigma) := \frac{1}{N}\sum_{i=1}^{N} \sigma_i$ as $H_N(\sigma) = -\frac{N}{2} m_N(\sigma)^2$.

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$m_N(k) = m_N(\sigma(k))$ is a Markov chain on $I_N = \{-1, -1+\frac{2}{N}, ..., 1-\frac{2}{N}, 1\}$ given by the transition probabilities

$$r(m, m') = \begin{cases} \frac{1-m}{2} \exp\left(-\frac{\beta N}{2}(m^2 - m'^2)_+\right) & \text{if } m' = m + \frac{2}{N} \\ \frac{1+m}{2} \exp\left(-\frac{\beta N}{2}(m^2 - m'^2)_+\right) & \text{if } m' = m - \frac{2}{N} \\ 1 - r\left(m, m+\frac{2}{N}\right) - r\left(m, m-\frac{2}{N}\right) & \text{if } m' = m \\ 0 & \text{otherwise.} \end{cases}$$

Phase transition

The process $t \mapsto m_N(\lfloor Nt \rfloor)$ weakly converges to the solution $m(t)$ of the ODE

$$\frac{d}{dt}m(t) = \left(e^{-2\beta(-m(t))_+} - e^{-2\beta(m(t))_+}\right) - m\left(e^{-2\beta(-m(t))_+} + e^{-2\beta(m(t))_+}\right).$$

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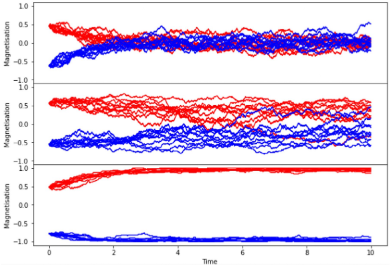

Figure: $\beta = 0.5$, $\beta = 1$, $\beta = 2$

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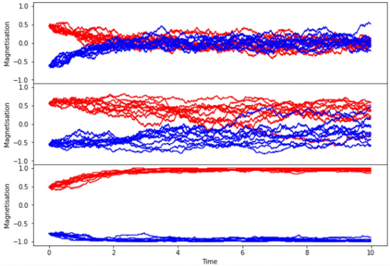

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Proof : consider the generator of $t \mapsto m_N(\lfloor Nt \rfloor)$ and show its convergence to the generator associated to the ODE.

II.2 ...with the Random Batch Method

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Consider again the sequence $m_{p,N}(k) = \frac{1}{N} \sum_i \sigma(k)_i$.

Transition probabilities

Lemma

In a system of size N, the transition probabilities for the magnetization with random batches of size p are given by

$$r_p(m,m') = \begin{cases} \frac{1-m}{2}\binom{N-1}{p-1}^{-1}\sum_{k=0}^{p-1}\binom{\left(\frac{1-m}{2}\right)N-1}{k}\binom{\left(\frac{1+m}{2}\right)N}{p-1-k}e^{-2\beta\left(\frac{2k+1-p}{p}\right)_+} & \text{if } m' = m+\frac{2}{N} \\ \frac{1+m}{2}\binom{N-1}{p-1}^{-1}\sum_{k=0}^{p-1}\binom{\left(\frac{1-m}{2}\right)N}{k}\binom{\left(\frac{1+m}{2}\right)N-1}{p-1-k}e^{-2\beta\left(\frac{p-1-2k}{p}\right)_+} & \text{if } m' = m-\frac{2}{N} \\ 1-r_p\left(m,m+\frac{2}{N}\right)-r_p\left(m,m-\frac{2}{N}\right) & \text{if } m' = m \\ 0 & \text{otherwise.} \end{cases}$$

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For instance

$$r_p\left(m,m+\frac{2}{N}\right) = \frac{1-m}{2}\frac{1}{\binom{N-1}{p-1}}\sum_{k=0}^{p-1}\binom{\left(\frac{1-m}{2}\right)N-1}{k}\binom{\left(\frac{1+m}{2}\right)N}{p-1-k}e^{-2\beta\left(\frac{2k+1-p}{p}\right)_+}$$

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$$r_p\left(m, m+\frac{2}{N}\right) = \overbrace{\frac{1-m}{2}}^{\text{Proportion of -1}} \frac{1}{\binom{N-1}{p-1}} \sum_{k=0}^{p-1}\left(\binom{\left(\frac{1-m}{2}\right)N-1}{k}\right)\left(\binom{\left(\frac{1+m}{2}\right)N}{p-1-k}\right)e^{-2\beta\left(\frac{2k+1-p}{p}\right)_+}$$

Transition probabilities

Lemma

In a system of size N, the transition probabilities for the magnetization with random batches of size p are given by

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For instance

$$r_p\left(m, m+\frac{2}{N}\right) = \frac{\overbrace{1-m}^{\text{Proportion of -1}}}{2}\ \underbrace{\frac{1}{\binom{N-1}{p-1}}}_{\#\text{ of clusters}}\ \overbrace{\sum_{k=0}^{p-1}\binom{\left(\frac{1-m}{2}\right)N-1}{k}\binom{\left(\frac{1+m}{2}\right)N}{p-1-k}}^{\text{Classifying the clusters based on the number of -1}}\ \underbrace{e^{-2\beta\left(\frac{2k+1-p}{p}\right)_+}}_{\text{Proba of changing}}$$

Limit ODE

The process $M_t^{(N,p)} = m_{N,p}(\lfloor Nt \rfloor)$ weakly converges as $N \to \infty$ to the solution of

$$\frac{d}{dt} m(t) = f_p(\beta, m(t)).$$

with $f_p(\beta, m) = \left(S_1^{p,\beta}(m) - S_2^{p,\beta}(m)\right) - m\left(S_1^{p,\beta}(m) + S_2^{p,\beta}(m)\right)$ where

$$S_1^{p,\beta}(m) = \mathbb{E}\left(e^{-2\beta\left(\frac{2X_{m,p}+1-p}{p}\right)_+}\right), \quad S_2^{p,\beta}(m) = \mathbb{E}\left(e^{-2\beta\left(\frac{p-1-2X_{m,p}}{p}\right)_+}\right)$$

$$\text{and} \quad X_{m,p} \sim \mathcal{B}\left(p-1, \frac{1-m}{2}\right).$$

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$$\text{and} \quad X_{m,p} \sim \mathcal{B}\left(p-1, \frac{1-m}{2}\right).$$

Recall the limit with no random batches

$$\frac{d}{dt} m(t) = \left(e^{-2\beta(-m(t))_+} - e^{-2\beta(m(t))_+}\right) - m\left(e^{-2\beta(-m(t))_+} + e^{-2\beta(m(t))_+}\right).$$

Decreased critical temperature

Theorem

Let $p \in \mathbb{N} \setminus \{0, 1\}$ *and* $\beta > 0$*.*

- *For all* $\beta > 0$, 0 *is an equilibrium state for the solution of the timit ODE.*
- *For* $p \in \{2, 3\}$, 0 *is the unique equilibrium state, and it is stable.*
- *For* $p \geq 4$*, there exists* $\beta_{c,p}$ *such that for all* $\beta > \beta_{c,p}$*, the equilibrium state 0 is unstable, and for all* $\beta \leq \beta_{c,p}$ *it is stable. Furthermore, we have the estimate*

$$\beta_{c,p} = 1 + \sqrt{\frac{2}{p\pi}} + o\left(\frac{1}{\sqrt{p}}\right).$$

Decreased critical temperature

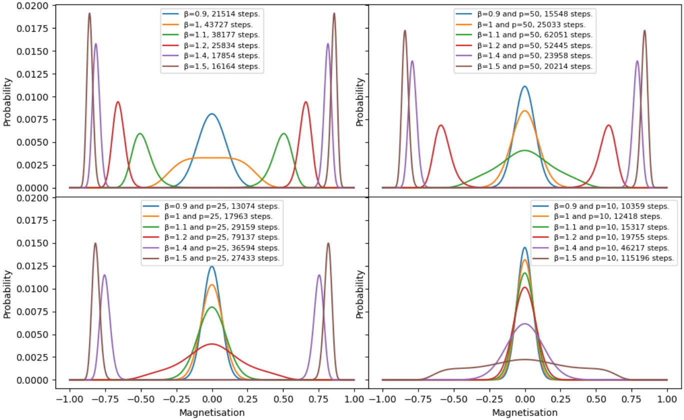

Figure: Numerical observation of the invariant distribution for the Curie-Weiss model

III. Double well potential

Double well potential

Consider in dimension one

$$\begin{cases} d\bar{X}_t = -U'(\bar{X}_t)dt - W' * \bar{\rho}_t(\bar{X}_t)dt + \sqrt{2\sigma}dB_t, \\ \bar{\rho}_t = \text{Law}(\bar{X}_t), \end{cases} \tag{DW-NL}$$

with the potentials

$$U(x) = \frac{x^4}{4} - \frac{x^2}{2}, \quad W(x) = L_W \frac{x^2}{2} \quad \text{with } L_W > 0.$$

Theorem (Tugaut '14)

There exists $\sigma_c > 0$ such that

- *For all $\sigma \geq \sigma_c$, there exists a unique stationary distribution $\mu_{\sigma,0}$ for* (DW-NL)*. Furthermore, $\mu_{\sigma,0}$ is symmetric.*
- *For all $\sigma < \sigma_c$, there exist three stationary distributions for* (DW-NL)*. One is symmetric, also denoted $\mu_{\sigma,0}$, and the other two, denoted $\mu_{\sigma,+}$ and $\mu_{\sigma,-}$, satisfy $\pm \int x d\mu_{\sigma,\pm}(dx) > 0$.*

Double well potential - Effective

$$\begin{cases} d\bar{X}_t = -U'(\bar{X}_t)dt - W' * \bar{\rho}_t(\bar{X}_t)dt + \left(2\sigma + \frac{\delta}{p-1} L_W^2 \text{Var}(\bar{\rho}_t)\right)^{1/2} dB_t, \\ \bar{\rho}_t = \text{Law}(\bar{X}_t), \end{cases} \tag{DW-Eff}$$

Theorem

For δ/p sufficiently small, denoting

$$\sigma_c^{eff} = \sigma_c \left(1 - \frac{\delta L_W}{2(p-1)}\right),$$

we have the following phase transition for the dynamics (DW-Eff)

- *For all $\sigma \geq \sigma_c^{eff}$, there exists a unique stationary distribution $\mu_{\sigma,0}^{\delta,p}$ for* (Eff)*. Furthermore, $\mu_{\sigma,0}^{\delta,p}$ is symmetric.*
- *For all $\sigma \in [\sigma_0, \sigma_c^{eff}[$, there exists exactly three stationary distributions for* (Eff)*. One is symmetric, also denoted $\mu_{\sigma,0}^{\delta,p}$, and the other two, denoted $\mu_{\sigma,+}^{\delta,p}$ and $\mu_{\sigma,-}^{\delta,p}$, satisfy $\pm \int x d\mu_{\sigma,\pm}^{\delta,p}(x) > 0$.*

Idea of proof

- Show that a stationary distribution for (DW-NL) is a stationary distribution for (DW-Eff), but for another diffusion coefficient.
- Study the variance around the critical parameter.

Merci