



Rigorous Evidence for Information-Computation Trade-offs, Sep. 2021

TO BE (HARD) OR NOT BE: THE SPIKED MATRIX-TENSOR MODEL

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GENERIC QUESTIONS:

For high-dimensional non-convex learning problems:

- How hard is it to sampling from the posterior ?
- How hard is it to compute the ML estimate?
- How does the energy/loss landscape affect the behaviour of gradient descent & sampling algorithms?
- Does the presence of spurious minima matter?
- How these approaches compare with message passing?

IN THIS TALK

An attempt to answer these questions in a simple yet generic problem

A synthetic problems where the <u>optimal</u> <u>performances</u> can be determined, the <u>energy landscape</u> characterised, and the behaviour of many algorithms (Message passing, Sampling, Gradient descent) analysed ...



The Matrix-Tensor spiked model on the sphere

SPIKED MATRIX-TENSOR PROBLEM

 $\mathbf{x}^* \in \mathbb{R}^N$

Choose a normed vector

 $\|\mathbf{x}^*\|_2^2 = \mathbf{N}$, randomly on the

sphere in N-dimension

W

Create a rank-noise noisy (symmetric) matrix

$$Y_{ij} = \frac{1}{\sqrt{N}} x_i^* x_j^* + \xi_{ij} \quad \xi_{ij} \sim \mathcal{N}(0, \Delta_2)$$

Create a rank-noise noisy (symmetric) tensor

$$T_{i_1...i_p} = \frac{\sqrt{(p-1)!}}{N^{(p-1)/2}} x_{i_1}^* \dots x_{i_p}^* + \xi_{i_1...i_p}$$

 $\xi_{i_1,\ldots,i_p} \sim \mathcal{N}(0,\Delta_p)$

Given the matrix T and the tensor Y, can one recover x*?

SPIKED MATRIX-TENSOR PROBLEM

• For the same signal \mathbf{x}^* in \mathbb{R}^N & observe a matrix Y <u>and</u> a tensor T:

$$Y = \frac{1}{\sqrt{N}} \mathbf{x}^* \mathbf{x}^* T + \sqrt{\Delta_2} W \qquad \qquad W_{ij} \sim \mathcal{N}(0,1)$$

$$T = \frac{\sqrt{(p-1)!}}{N^{(p-1)/2}} \mathbf{x}^{*\otimes p} + \sqrt{\Delta_p} Z$$

 $Z_{ijk} \sim \mathcal{N}(0,1)$

• Can one recover x* from T and Y?

SPIKED MATRIX-TENSOR PROBLEM PLANTED VERSION OF THE '2+P' SPIN GLASS IN STATISTICAL PHYSICS

• Define the Hamiltonian (or cost function):

$$\mathcal{H}(x) = -\frac{1}{\Delta_2 \sqrt{N}} \sum_{i < j} Y_{ij} x_i x_j - \frac{\sqrt{(p-1)!}}{\Delta_p N^{(p-1)/2}} \sum_{i_1 < \ldots < i_p} T_{i_1 \ldots i_p} x_{i_1} \ldots x_{i_p}$$

spherical constraint:
$$\sum_{i=1}^N x_i^2 = N$$

- Bayes-optimal estimation = marginals of Gibbs measure
 - $\hat{\mathbf{x}} = \mathbb{E}_{P(\mathbf{X}|Y,T)}[\mathbf{x}] \qquad P_{\text{Gibbs}}(\mathbf{x}|Y,T) = \frac{1}{Z(Y,T)}e^{-\mathcal{H}_{Y,T}(x)}$

• MMSE =
$$\|\hat{\mathbf{x}} - \mathbf{x}^*\|_2^2$$

[Derrida 81, Mezard-Gross '84, many others]

SPIKED MATRIX-TENSOR PROBLEM PLANTED VERSION OF THE '2+P' SPIN GLASS IN STATISTICAL PHYSICS

• Define the Hamiltonian (or cost function):

$$\mathcal{H}(x) = -\frac{1}{\Delta_2 \sqrt{N}} \sum_{i < j} Y_{ij} x_i x_j - \frac{\sqrt{(p-1)!}}{\Delta_p N^{(p-1)/2}} \sum_{i_1 < \ldots < i_p} T_{i_1 \ldots i_p} x_{i_1} \ldots x_{i_p}$$

spherical constraint:
$$\sum_{i=1}^N x_i^2 = N$$

• Maximum likelihood (MLE)

$$\mathscr{L}(\mathbf{x}) = \frac{1}{2\Delta_2} \|Y - \frac{\mathbf{x}\mathbf{x}^T}{\sqrt{N}}\|_2^2 + \frac{1}{p!\Delta_p} \|T - \sqrt{(p-1)!}\frac{\mathbf{x}^{\otimes p}}{N^{(p-1)/2}}\|_2^2$$

Minimize $\mathscr{L}(\mathbf{x})$ subject to $\|\mathbf{x}\|_2^2 = N$



Computational-Statistical Gaps: What do we know?

$$P_{\text{Gibbs}}(\mathbf{x} \mid Y, T) = \frac{1}{Z(Y, T)} e^{-\mathcal{H}_{Y,T}(x)}$$

From the free energy, $\frac{1}{N} \log Z(Y)$, we can compute *anything*

Mutual Information

$$\frac{I(X;Y)}{N} = \frac{(\mathbb{E}[X^2])^2}{4\Delta} - \mathbb{E}_Y \left[\frac{1}{N}\log Z(Y)\right]$$

$$\frac{1}{1}\log\left(\frac{P_{\text{spiked}}(Y)}{1}\right) = \frac{1}{1}\log Z(Y)$$

Likelihood ratio

$$\frac{1}{N} \log \left(\frac{P_{\text{spiked}}(Y)}{P_{\text{null}}(Y)} \right) = \frac{1}{N} \log Z(Y)$$

Kullback-Leibler

 $D_{\mathrm{KL}}(P_{\mathrm{Spiked}} || P_{\mathrm{Null}}) = \mathbb{E}_{Y} \log Z(Y)$

Theorem 1 (informally): "replica symmetric potential"

For large N, $\frac{1}{N} \log Z(Y, \Delta)$ concentrates around the max of $\Phi_{RS}(m)$ $\Phi_{RS} = \frac{1}{2} \log(1-m) + \frac{m}{2} + \frac{m^2}{4\Delta_2} + \frac{m^p}{2p\Delta_p}$ $m \in [0,1]$

[Mannelli, Biroli, Cammarota, FK, Urbani, & Zdeborová '18]

Theorem 1 (informally): "replica symmetric potential"



[Mannelli, Biroli, Cammarota, FK, Urbani, & Zdeborová '18]



WHAT ARE THE BEST ALGORITHMS SO FAR?

APPROXIMATE MESSAGE PASSING AN ITERATIVE THRESHOLDING ALGORITHM

Approximate Message Passing

$$\begin{split} \mathbf{B}^{(2,t)} &= \frac{1}{\Delta_2 \sqrt{N}} Y \hat{\mathbf{x}}^t - \frac{1}{\Delta_2} \hat{\sigma}^t \hat{\mathbf{x}}^{t-1} \\ \mathbf{B}^{(p,t)} &= \frac{\sqrt{(p-1)!}}{\Delta_p N^{(p-1)/2}} T(\hat{\mathbf{x}}^t)^{\otimes p-1} - \frac{p-1}{\Delta_p} \hat{\sigma}^t \left[\frac{(\hat{\mathbf{x}}^t) \cdot (\hat{\mathbf{x}}^{t-1})}{N} \right]^{p-2} \hat{\mathbf{x}}^{t-1} \\ A^{(2,t)} &= \frac{\|\hat{\mathbf{x}}^t\|_2^2}{\Delta_2 N} \qquad A^{(p,t)} = \frac{(\|\hat{\mathbf{x}}^t\|_2^2)^{p-1}}{\Delta_p N} \\ \hat{\mathbf{x}}^{t+1} &= \eta (A^{(2,t)} + A^{(p,t)}, \mathbf{B}^{(2,t)} + \mathbf{B}^{(p,t)}) \qquad \eta(A,B) = \frac{B}{1+A} \\ \hat{\sigma}^{t+1} &= \frac{1}{1+A^{(2,t)} + A^{(p,t)}} \end{split}$$

[Montanari, Richard '15; Mannelli, Biroli, Cammarota, FK, Urbani, & Zdeborová '18]

THE HARD PHASE OF AMP



TWO LIMITS



TWO LIMITS



TWO LIMITS



THE HARD PHASE OF AMP



WHAT ABOUT PRACTICAL OFF-THE-SHELVES ALGORITHMS?

Sampling the posterior with MCMC or Langevin?

MLE with gradient descent?

Connection gradient descent with property of the landscapes?

Presence/Absence of spurious minima?

All these can be studied analytically & quantitively in the spherical spiked matrix-tensor model



Sampling the posterior with Langevin dynamics

LANGEVIN ALGORITHM

spherical constraint

$$\dot{x}_i(t) = -\mu(t)x_i(t) - \frac{\partial \mathcal{H}}{\partial x_i} + \eta_i(t)$$

gradient
 $\langle \eta_i(t)\eta_j(t') \rangle = 2\delta_{ij}\delta(t-t')$
 $T=1 \text{ noise}$

At large time (exponential in N) samples the posterior measure. Where does it go in large but constant time?

Analytical solution of the off-equilibrium dynamics of a long-range spin-glass model

L. F. Cugliandolo and J. Kurchan Phys. Rev. Lett. **71**, 173 – Published 5 July 1993

Zeitschrift für Physik B Condensed Matter

A. Crisanti, H. Horner, H. -J. Sommers

June 1993, Volume 92, <u>Issue 2</u>, pp 257–271 | <u>Cite as</u>

Article

The spherical*p*-spin interaction spin-glass model

The dynamics

Authors

Authors and affiliations

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From

CUGLIANDOLO-KURCHAN EQUATIONS FOR DYNAMICS OF SPIN-GLASSES.

GERARD BEN AROUS, AMIR DEMBO, AND ALICE GUIONNET

ABSTRACT. We study the Langevin dynamics for the family of spherical p-spin disordered meanfield models of statistical physics. We prove that in the limit of system size N approaching infinity, the empirical state correlation and integrated response functions for these N-dimensional coupled diffusions converge almost surely and uniformly in time, to the non-random unique strong solution of a pair of explicit non-linear integro-differential equations, first introduced by Cugliandolo and Kurchan.

Probability Theory and Related Fields 136, 619–660 (2006)

ITHM

LANGEVIN STATE EVOLUTION

$$C_{N}(t,t') \equiv \frac{1}{N} \sum_{i=1}^{N} x_{i}(t) x_{i}(t') ,$$

$$\overline{C}_{N}(t) \equiv \frac{1}{N} \sum_{i=1}^{N} x_{i}(t) x_{i}^{*} , = m_{\text{Langevin}}(t)$$

$$R_{N}(t,t') \equiv \frac{1}{N} \sum_{i=1}^{N} \partial x_{i}(t) / \partial h_{i}(t')|_{h_{i}=0} ,$$

$$\begin{split} &\frac{\partial}{\partial t}C(t,t') = 2R(t',t) - \mu(t)C(t,t') + Q'(\overline{C}(t))\overline{C}(t') + \int_0^t dt'' R(t,t'')Q''(C(t,t''))C(t',t'') + \int_0^{t'} dt'' R(t',t'')Q'(C(t,t'')) \\ &\frac{\partial}{\partial t}R(t,t') = \delta(t-t') - \mu(t)R(t,t') + \int_{t'}^t dt'' R(t,t'')Q''(C(t,t''))R(t'',t') \,, \\ &\frac{\partial}{\partial t}\overline{C}(t) = -\mu(t)\overline{C}(t) + Q'(\overline{C}(t)) + \int_0^t dt'' R(t,t'')\overline{C}(t'')Q(C(t,t'')) \,, \\ &Q(x) = x^2/(2\Delta_2) + x^p/(p\Delta_p) \,. \end{split}$$

Generalization of the CHSCK equations that includes the spike x*. [Mannelli, Biroli, Cammarota, FK, Urbani, & Zdeborová '18]

LANGEVIN STATE EVOLUTION (NUMERICAL SOLUTION)



http://github.com/sphinxteam/spiked_matrix-tensor

AMP SAMPLNG VS LANGEVIN SAMPLING

OK, Langevin is *slower*....

... but does it work as well as AMP in the long run (i.e linear but large time)?



LANGEVIN STATE EVOLUTION (NUMERICAL SOLUTION)



Figure 4: Correlation with the signal of AMP and Langevin at the kth iteration (at time t) for fixed $\Delta_2 = 0.7$.

http://github.com/sphinxteam/spiked_matrix-tensor

A LANGEVIN PHASE TRANSITION



AMP BEATS LANGEVIN

Langevin dynamics display **worst** performances w.r.t. Bayes-AMP

Physicists: "Residual glassiness prevents a correct sampling"

We expect the same picture to hold in all problems having hard phase associated to the first order phase transition. (e.g. GLM, Teacher-Student Neural networks, ...)

A PARISI-FRANZ VISION BEWARE: THIS SLIDE IS FOR REPLICA GEEKS

Consider the free energy of a system conditioned at a given overlap m from truth vector **x***



$$\Phi_{FP}(m) = \lim_{N \to \infty} \frac{1}{N} \mathbb{E}_{Y} \log Z(Y, m)$$
$$\log Z(Y, m) = \int d\mathbf{x} e^{-\mathcal{H}} \mathbf{1} \left(\mathbf{m} - \frac{\mathbf{x} \cdot \mathbf{x}^{*}}{\mathbf{N}} \right)$$

AMP try to optimize the Replica-Symetric potentiel

[Antenucci, Franz, Urbani, Zdeborova '19]

Langevin try to optimize the Actual (RSB) potential



MLE, Gradient & Landscapes

MLE AND MINIMIZATION

• For the same signal **x*** observe a matrix Y <u>and</u> a tensor T as:

$$Y_{ij} = \frac{1}{\sqrt{N}} x_i^* x_j^* + \xi_{ij} \qquad \xi_{ij} \sim \mathcal{N}(0, \Delta_2)$$

$$T_{i_1 \dots i_p} = \frac{\sqrt{(p-1)!}}{N^{(p-1)/2}} x_{i_1}^* \dots x_{i_p}^* + \xi_{i_1 \dots i_p} \qquad \xi_{i_1, \dots, i_p} \sim \mathcal{N}(0, \Delta_p)$$

• Maximum likelihood (MLE)

$$\mathscr{L}(\mathbf{x}) = \frac{1}{2\Delta_2} \|Y - \frac{\mathbf{x}\mathbf{x}^T}{\sqrt{N}}\|_2^2 + \frac{1}{2\Delta_p} \|T - \sqrt{(p-1)!}\frac{\mathbf{x}^{\otimes p}}{N^{(p-1)/2}}\|_2^2$$

Minimize $\mathscr{L}(\mathbf{x})$ subject to $\|\mathbf{x}\|_2^2 = N$

GRADIENT FLOW ZERO TEMPERATURE LIMIT OF LANGEVIN

$$\dot{x}_{i}(t) = -\mu(t)x_{i}(t) - \frac{\partial\mathcal{H}}{\partial x_{i}} + \eta_{i}(t)$$
$$\dot{x}_{i}(t) = -\mu(t)x_{i}(t) - \frac{\partial\mathcal{H}}{\partial x_{i}}$$

Can be analysed again with the Langevin State evolution Simply the T \rightarrow 0 limit of the CHSCK equations

LANGEVIN STATE EVOLUTION ZERO TEMPERATURE LIMIT: GRADIENT FLOW

$$C_N(t,t') \equiv \frac{1}{N} \sum_{i=1}^N x_i(t) x_i(t') ,$$

$$\overline{C}_N(t) \equiv \frac{1}{N} \sum_{i=1}^N x_i(t) x_i^* , = m_{\text{GD}}(t)$$

$$R_N(t,t') \equiv \frac{1}{N} \sum_{i=1}^N \partial x_i(t) / \partial h_i(t')|_{h_i=0} ,$$

$$\begin{split} \frac{\partial}{\partial t} C(t,t') &= -\tilde{\mu}(t)C(t,t') + Q'(m(t))m(t') + \int_0^t dt'' R(t,t'')Q''(C(t,t''))C(t',t'') \\ &+ \int_0^{t'} dt'' R(t',t'')Q'(C(t,t'')) \,, \\ \frac{\partial}{\partial t} R(t,t') &= -\tilde{\mu}(t)R(t,t') + \int_{t'}^t dt'' R(t,t'')Q''(C(t,t''))R(t'',t') \,, \\ \frac{\partial}{\partial t} m(t) &= -\tilde{\mu}(t)m(t) + Q'(m(t)) + \int_0^t dt'' R(t,t'')m(t'')Q(C(t,t'')) \,, \end{split}$$

 $Q(x) = \frac{x^2}{(2\Delta_2)} + \frac{x^p}{(p\Delta_p)}.$

[Mannelli, Biroli, Cammarota, FK, Urbani, & Zdeborová '18]

NUMERICAL INTEGRATION



ANALYTICAL SOLUTION (LONG TIME EXTRAPOLATION)



ENERGY LANDSCAPE

• Maximum likelihood (MLE)

$$\mathscr{L}(\mathbf{x}) = \frac{1}{2\Delta_2} \| Y - \frac{\mathbf{x}\mathbf{x}^T}{\sqrt{N}} \|_F^2 + \frac{1}{p!\Delta_p} \| T - \sqrt{(p-1)!} \frac{\mathbf{x}^{\otimes p}}{N^{(p-1)/2}} \|_F^2$$

Minimize $\mathscr{L}(\mathbf{x})$ subject to $\|\mathbf{x}\|_2^2 = N$

- Can we compute the property of the energy landscape ?
- Number of minimas/saddles at each energy level?
- Are the minima spurious or good ones?

LANDSCAPE & MINIMAS THE KAC-RICE FORMULA

$$\lim_{N \to \infty} \frac{1}{N} \log \mathbb{E} \left[\mathcal{N}(m, \epsilon_2, \epsilon_p) \right] = \tilde{\Sigma}_{\Delta_2, \Delta_p}(m, \epsilon_2, \epsilon_p)$$

$$\mathcal{N}(m,\epsilon_2,\epsilon_p;\Delta_2,\Delta_p) = e^{\tilde{\Sigma}_{\Delta_2,\Delta_p}(m,\epsilon_2,\epsilon_p)} = \int_{\mathbb{S}^{N-1}} \mathbb{E}[\det H|G=0, F_2=N\epsilon_2, F_p=N\epsilon_p, H \succ 0]\phi_{G,F_2,F_p}(\sigma,0,\epsilon_2,\epsilon_p)\,\delta(m-\sigma\cdot\sigma^*)\,\mathrm{d}\sigma$$

[Fyodorov Y. V. '03; Auffinger A., Ben Arous G., & Cerny J '13]

LANDSCAPE & MINIMAS KAC-RICE FOR THE SPIKE MODEL

$$\lim_{N \to \infty} \frac{1}{N} \log \mathbb{E} \left[\mathcal{N}(m, \epsilon_2, \epsilon_p) \right] = \tilde{\Sigma}_{\Delta_2, \Delta_p}(m, \epsilon_2, \epsilon_p)$$

$$\tilde{\Sigma}_{\Delta_{2},\Delta_{p}}(m,\epsilon_{2},\epsilon_{p}) = \frac{1}{2}\log\frac{\frac{p-1}{\Delta_{p}} + \frac{1}{\Delta_{2}}}{\frac{1}{\Delta_{p}} + \frac{1}{\Delta_{2}}} + \frac{1}{2}\log(1-m^{2}) - \frac{1}{2}\frac{\left(\frac{m^{p-1}}{\Delta_{p}} + \frac{m}{\Delta_{2}}\right)^{2}}{\frac{1}{\Delta_{p}} + \frac{1}{\Delta_{2}}}(1-m^{2}) - 2p\Delta_{p}\left(\epsilon_{p} - \frac{m^{p}}{2p\Delta_{p}}\right)^{2} - 4\Delta_{2}\left(\epsilon_{2} - \frac{m^{2}}{4\Delta_{2}}\right)^{2} + \Phi(t) - L(\theta,t),$$

$$\Phi(t) = \frac{t^2}{4} + \mathbb{1}_{|t|>2} \left[\log\left(\sqrt{\frac{t^2}{4} - 1} + \frac{|t|}{2}\right) - \frac{|t|}{4}\sqrt{t^2 - 4} \right]$$

$$L(\theta, t) = \begin{cases} \frac{1}{4} \int_{\theta + \frac{1}{\theta}}^t \sqrt{y^2 - 4} dy - \frac{\theta}{2} \left(t - \left(\theta + \frac{1}{\theta}\right)\right) + \frac{t^2 - \left(\theta + \frac{1}{\theta}\right)^2}{8} & \theta > 1, \ 2 \le t < \frac{\theta^2 + 1}{\theta} \\ \infty & t < 2 \\ 0 & \text{otherwise.} \end{cases}$$

(Note: we also checked that annealed is equal to quenched, thanks to the replica method)

[Ben Arous, Mei, Montanari, & Nica '17, Sarao, FK, Urbani & Zdeborova '19]

LANDSCAPE ANALYSIS

(exponentially many saddles points)

V V V V V V V V V V V V V V V

energy

Low SNR / large noise situation

Similar as in Levent, Guney, Ben Arous & LeCun '14

LANDSCAPE ANALYSIS



WHAT IS ACTUALLY GOING ON



LANDSCAPE ANA

THE

TEOFTHE

Trivialisation

energy V V V VV V VV V VVV VV V V

Increasing the SNR

LANDSCAPE ANALYSIS



Increasing the SNR

ANALYTICAL SOLUTION (LANDCSAPE ANALYSIS)



IN A NUTSHELL



CONCLUSIONS...

- Spherical spike matrix-tensor problem has interesting properties; Many quantities can be computed (*Optimal performances, energy landscape, performance of AMP, Langevin, Gradient descent...*)
- Observed Gap between Langevin sampling and message passing performances: MCMC not as good as Langevin?
- Minimisation algorithms are observed to work just fine even in presence of (exponentially many) spurious minima

... PERSPECTIVES?

- More on monte-carlo sampling in M. C. Angelini's talk tomorrow
- Other non convex learning and signal processing problems (e.g. Phase retrieval, see Antoine Maillard's talk tomorrow)
- Effect of prior information (see Bruno Loureiro's talk next)
- Neural networks: Single layer perceptron, teacher-student multilayer deep networks, over-parametrization, etc...
- Non convex setting with other gradient-based algorithms SGD, Nesterov, momentum, etc, (Recent papers by Zdeborova, Mignacco, Urbani...)

REFERENCES FOR THIS TALK

- Marvels and pitfalls of the Langevin algorithm in noisy highdimensional inference; Sarao, Biroli, Cammarota, FK, Urbani, Zdeborova, PRX '19.
- Passed & Spurious: Descent Algorithms and Local Minima in Spiked Matrix-Tensor Models; Sarao, FK, Urbani, Zdeborova, ICML'19, arXiv:1902.00139.
- Who is Afraid of Big Bad Minima? Analysis of Gradient-Flow in a Spiked Matrix-Tensor Model; Sarao, Biroli, Cammarota, FK, Urbani, Zdeborova. **NeurIPS '19**.



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