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TAP equations are repulsive*

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Abstract

We show that for low enough temperatures, but still above the AT line, the Jacobian of the TAP equations for the SK model has a macroscopic fraction of eigenvalues outside the unit interval. This provides a simple explanation for the numerical instability of the fixed points, which thus occurs already in high temperature. The insight leads to some algorithmic considerations on the low temperature regime.

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1 Introduction

Consider $N \in \mathbb{N}, \beta > 0, h \in \mathbb{R}$, and independent standard Gaussians $\boldsymbol{g} = (g_{ij})_{1 \le i < j \le N}$ issued on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The TAP equations [17] for the spin magnetizations $\boldsymbol{m} = (m_i)_{i=1}^N \in [-1,1]^N$ in the SK-model [10] at inverse temperature β and external field h read

$$m_i = \tanh\left(h + \frac{\beta}{\sqrt{N}} \sum_{j:j\neq i} g_{ij} m_j - \beta^2(1-q) m_i \right), \quad i = 1, \dots, N, \tag{1.1}$$

where we set $g_{ij} = g_{ji}$ for $i > j$. The β^2-term is the (limiting) Onsager correction: it involves the *high temperature* order parameter q which is the (for $\beta \le 1$ or $h \neq 0$ unique, see [11, Proposition 1.3.8]) solution of the fixed point equation

$$q = \mathsf{E} \tanh^2\left(h + \beta\sqrt{q} Z\right), \tag{1.2}$$

Z being a standard Gaussian, and E its expectation. The concept of *high temperature* is related to the AT-line [2], the (β, h)-region satisfying

$$\beta^2 \mathsf{E} \frac{1}{\cosh^4(h + \beta\sqrt{q}Z)} = 1. \tag{1.3}$$

For (β, h) where the l.h.s. is strictly less than unity, the system is allegedly in the replica symmetric phase (high temperature), see e.g. Adhikari *et.al.* [1] for a recent thorough discussion of this issue, and Chen [8] for evidence supporting the conjecture.

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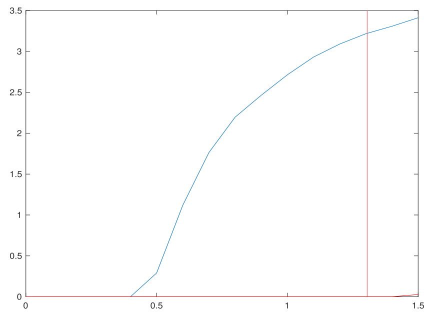


Figure 1: To illustrate: MSE (y-axis) between (the last) two iterates as a function of β (x-axis), to fixed magnetic field $h = 0.3$, and one single realization of the disorder. System size $N = 250$. We have run Banach algorithm $k = 1000$ times, randomly initialized (uniformly chosen $\boldsymbol{m}^{(0)}$). Visibly, iterations stabilize for small β, but diverge beyond the threshold ≈ 0.4, way below the AT-line (red). The red flat line (essentially coinciding with the x-axis) is Bolthausen's algorithm, which clearly converges below AT.

Due to the fixed point nature of the TAP equations (1.2), one is perhaps tempted to solve them numerically via classical Banach iterations, i.e. to approximate solutions via

$$m_i^{(k+1)} = \tanh\left(h + \frac{\beta}{\sqrt{N}} \sum_{j: j \neq i} g_{ij} m_j^{(k)} - \beta^2 (1-q) m_i^{(k)} \right), \quad i = 1, \dots, N. \tag{1.4}$$

As it turns out, these plain iterations are astonishingly *in*-efficient in finding stable fixed points[1] insofar the mean squared error between two iterates, to wit:

$$\text{MSE}\left(\boldsymbol{m}^{(k+1)}, \boldsymbol{m}^{(k)}\right) \equiv \frac{1}{N} \sum_{i=1}^{N} \left(m_i^{(k+1)} - m_i^{(k)} \right)^2, \tag{1.5}$$

often remains large, even for very large $k's$. Even more surprising, this issue is not restricted to the low temperature phase, cfr. Figure 1 above.

Bolthausen [5] bypasses this problem by a modified Banach algorithm (recalled below) which converges up to the AT-line. Notwithstanding, the origin of the phenomenon captured by Figure 1 has not yet been, to our knowledge, identified. It is the purpose of this work to fill this gap. Precisely, we show in Theorem 1 below that classical Banach iterates become unstable for the simplest reason, namely for large enough β, but still below the AT-line, iterates of TAP equations become repulsive: they do not stabilize. This should be contrasted with the classical counterpart of the SK-model: it is well known (and a simple fact) that *relevant* solutions of the fixed point equations for the Curie-Weiss model are attractive at *any* temperature, with the *irrelevant* solution even becoming repulsive in low temperature.

2 Main result

2.1 Iterative procedure for the magnetizations

Bolthausen [5] constructs magnetizations $\boldsymbol{m}^{(k)} = \left(m_i^{(k)}\right)_{i \leq N}$ for given disorder $(g_{ij})_{1 \leq i < j \leq N}$ through an iterative procedure in $k = 1, 2, \dots$. These magnetizations approximate fixed points of the TAP equations in the limit $N \to \infty$ followed by $k \to \infty$. The algorithm uses the initial values $\boldsymbol{m}^{(0)} = \mathbf{0}$, $\boldsymbol{m}^{(1)} = \sqrt{q}\mathbf{1}$. The iteration step reads

$$m_i^{(k+1)} = \tanh\left(h + \frac{\beta}{\sqrt{N}} \sum_{j:\, j \neq i} g_{ij} m_j^{(k)} - \beta^2 (1-q) m_i^{(k-1)} \right), \tag{2.1}$$

[1] this observation has been made, at times anecdotally, ever since: it is already present in Mézard, Parisi and Virasoro [12, Section II.4].

for $i \leq N$, and $k \in \mathbb{N}$. Remark in particular that contrary to the classical Banach algorithm, the above scheme invokes a time delay in the Onsager correction: we will thus refer to (2.1) as *Two Steps Banach algorithm*, 2SteB for short. By [5, Proposition 2.5], the quantity $q_N := N^{-1}\sum_{i=1}^N (m_i^{(k)})^2$ converges to q in probability and in expectation, as $N \to \infty$ followed by $k \to \infty$. Moreover, by [5, Theorem 2.1],

$$\lim_{k,k'\to\infty} \limsup_{N\to\infty} \mathbb{E}\left[\frac{1}{N}\sum_{i=1}^N \left(m_i^{(k)} - m_i^{(k')}\right)^2\right] = 0, \tag{2.2}$$

provided (β, h) is below the AT-line, i.e. if the left-hand side of (1.3) is less than unity.

2.2 Spectrum of the Jacobian

Denote by $F_i(\boldsymbol{m}^{(k)})$ the right-hand side of (1.4), and consider the matrix

$$J_{ij}^{(k)} := \frac{\partial F_i}{\partial m_j}(\boldsymbol{m}^{(k)}) = \begin{cases} \frac{\beta}{\sqrt{N}} g_{ij}\left(1 - F_i\left(\boldsymbol{m}^{(k)}\right)^2\right) : i \neq j \\ -\beta^2(1-q)\left(1 - F_i\left(\boldsymbol{m}^{(k)}\right)^2\right) : i = j, \end{cases} \tag{2.3}$$

omitting the obvious N-dependence to lighten notations. $J^{(k)}$ is not symmetric, but we claim that it is nonetheless diagonalizable, and that all eigenvalues are real. To see this we write the Jacobian as a product

$$J^{(k)} = \mathrm{diag}\left(1 - F_\cdot\left(\boldsymbol{m}^{(k)}\right)^2\right)\hat{J}, \tag{2.4}$$

where

$$\hat{J}_{ij} := \begin{cases} \frac{\beta}{\sqrt{N}} g_{ij} & i \neq j, \\ -\beta^2(1-q) & i = j. \end{cases} \tag{2.5}$$

The first matrix on the r.h.s. of (2.4) is positive definite whereas the second is symmetric: with $A := J^{(k)}$ and $S := \mathrm{diag}\left(1 - F_\cdot\left(\boldsymbol{m}^{(k)}\right)^2\right)$ it follows that

$$AS = \mathrm{diag}\left(1 - F_\cdot\left(\boldsymbol{m}^{(k)}\right)^2\right)\hat{J}\mathrm{diag}\left(1 - F_\cdot\left(\boldsymbol{m}^{(k)}\right)^2\right) = SA^t, \tag{2.6}$$

and therefore it follows from [9, Theorem 1] that $A = J^{(k)}$ itself is diagonalizable, and that all its eigenvalues are real, settling our claim.

Denoting the ordered sequence of the real eigenvalues of a matrix M by $\lambda_1(M) \geq \ldots \geq \lambda_N(M)$, we then consider the empirical spectral measure of the Jacobian

$$\mu^{(k)} := \frac{1}{N}\sum_{i=1}^N \delta_{\lambda_i(J^{(k)})}. \tag{2.7}$$

Our main result[2] states that in a region below the AT-line, $\mu^{(k)}$ has mass outside the unit interval.

Theorem 1. For all $\beta \in (\sqrt{2}-1, 1)$ and $\epsilon > 0$, there exist $h_0 > 0$, $\delta > 0$ such that the following holds true: for all $h \in [0, h_0]$, there exists $k_0 \in \mathbb{N}$, and for all $k \geq k_0$, there exists $N_0 \in \mathbb{N}$, such that $\mathbb{P}\left(\mu^{(k)}(-\infty, -1) > \delta\right) \geq 1 - \epsilon$, for all $N \geq N_0$.

[2] See also [7] for a treatment similar in spirit to our considerations, albeit with radically different tools, for $\mathbb{Z}_2$-synchronization.

Classical Banach iterations therefore stop to converge even below the AT-line due to a macroscopic fraction of low-lying (< -1) eigenvalues of the Jacobian. Before giving a proof of this statement, we remark that the measures $\mu^{(k)}$ converge to a limiting measure μ which can be stated as a free multiplicative convolution

$$\mu = \lambda_{\beta,q} \boxtimes \nu, \tag{2.8}$$

where $\lambda_{\beta,q}$ is the law of $\beta X - \beta^2(1-q)$ for X distributed according to the standard semicircular law with density $x \ni [-2,2] \mapsto (2\pi)^{-1}\sqrt{4-x^2}$, and ν is the law of $1 - \tanh^2(h + \beta\sqrt{q}Z)$ for Z standard Gaussian. To sketch a proof of this claim, we use the decomposition (2.4) and make the following observations: *i)* The empirical spectral distribution of the first factor $\hat{J}$ weakly-converges almost surely to the scaled/shifted semicircular law $\lambda_{\beta,q}$; *ii)* The empirical spectral distribution of the second factor $1 - F_{\cdot}(\boldsymbol{m}^{(k)})^2$ can similarly be shown to converge to ν. These observations, together with the (asymptotic) independence of the two factors which follows from [6], and finally [3, Theorem 5.4.2] then yield the representation (2.8).

The free convolution can also be evaluated more explicitly using Voiculescu's S-transform via inversion of moment generating functions, see e.g. [3, Chapter 5.3]. We believe this approach allows to remove the *small-h condition* in Theorem 1. The ensuing analysis is however both long and (tediously) technical. As the outcome arguably adds little to the main observation of this work, we refrain from pursuing this route here.

Proof of Theorem 1. We first consider a simplified version of the Jacobian, namely the matrix $\hat{J}$ from (2.5) in place of $J^{(k)}$. We write $\hat{J} = W - \beta^2(1-q)I$, where W is a Wigner matrix. As a consequence of Wigner's theorem, see e.g. [15, Theorem 2.4.2], the empirical spectral measure $\hat{\mu}$ associated with $\hat{J}$ converges a.s. with respect to the vague topology to the law of $\beta X - \beta^2(1-q)$, where X has the standard semicircular density. We note that this limit law has mass in any right vicinity of $-2\beta - \beta^2(1-q)$.

Next we show that $\mu^{(k)}$ and $\hat{\mu}$ converge to the same limit as $N \to \infty$ followed by $k \to \infty$, and finally $h \to 0$. To this aim, let $R^{(k)}(z) = (J^{(k)} - zI)^{-1}$ and $\hat{R}(z) = (\hat{J} - zI)^{-1}$ denote the resolvents of $J^{(k)}$ and $\hat{J}$, respectively. It suffices to show that the Stieltjes transforms $N^{-1}\mathrm{tr}\,\hat{R}(z)$ and $N^{-1}\mathrm{tr}\,R^{(k)}(z)$ of $\hat{\mu}$ and $\mu^{(k)}$, respectively, converge to the same limit in probability as $N \to \infty$ followed by $k \to \infty$ and $h \to 0$, pointwise for all $z \in \mathbb{C} \setminus \mathbb{R}$, see e.g. [3, Theorem 2.4.4]. By the resolvent identity,

$$N^{-1}\mathrm{tr}\,R^{(k)}(z) - N^{-1}\mathrm{tr}\,\hat{R}(z) = N^{-1}\mathrm{tr}\,R^{(k)}(z)\left(\hat{J} - J^{(k)}\right)\hat{R}(z). \tag{2.9}$$

The p-Schatten norm of an $N \times N$ matrix M whose eigenvalues are all real is defined by

$$\|M\|_p := \left(\sum_{i=1}^{N} |\lambda_i(M)|^p\right)^{1/p} \quad \text{for } p \in [1,\infty), \quad \|M\|_\infty := \max\{|\lambda_i(M)| : i = 1,\dots,N\} \tag{2.10}$$

which satisfies $\|M\|_1 \geq |\mathrm{tr}\,M|$ and the Hölder inequality. Hence, the expression in (2.9) is bounded in absolute value by

$$\|R^{(k)}(z)\|_\infty \|\hat{R}(z)\|_\infty \|\hat{J}\|_\infty N^{-1} \|\mathrm{diag} F_{\cdot}(\boldsymbol{m}^{(k)})^2\|_1, \tag{2.11}$$

where we evaluated $\hat{J} - J^{(k)}$ using (2.4). Each of the first two terms in (2.11) is bounded by $1/|\Im z|$, which follows from the definition of the resolvent. The third term $\|\hat{J}\|_\infty$ converges in probability to $2\beta + \beta^2(1-q)$ as $N \to \infty$. Indeed, the largest eigenvalue of $\hat{J}$ converges in probability to $2\beta - \beta^2(1-q)$, and the smallest to $-2\beta - \beta^2(1-q)$ (see e. g. [16, Theorem 1.13] and note that the Weyl inequalities [15, equation (1.5.4)], allow to consider $\hat{J} + \beta^2(1-q)$ as a Gaussian orthogonal ensemble, despite its zero diagonal elements). From the definitions of $F_i(\boldsymbol{m}^{(k)})$ and $m_i^{(k+1)}$, and as the function $x \mapsto \tanh^2(x)$ is 2-Lipschitz continuous,

$$\left|F_i(\boldsymbol{m}^{(k)})^2 - {m_i^{(k+1)}}^2\right| = \left|\tanh^2\left(h + \frac{\beta}{\sqrt{N}}\sum_{j:j\neq i} g_{ij} m_j^{(k)} - \beta^2(1-q)m_i^{(k)}\right)\right.$$
$$\left. - \tanh^2\left(h + \frac{\beta}{\sqrt{N}}\sum_{j:j\neq i} g_{ij} m_j^{(k)} - \beta^2(1-q)m_i^{(k-1)}\right)\right| \le 2\beta^2(1-q)\left|m_i^{(k)} - m_i^{(k-1)}\right|. \tag{2.12}$$

Hence, by definition of the 1-Schatten norm,

$$N^{-1}\|\mathrm{diag}F.(\boldsymbol{m}^{(k)})^2\|_1 \le N^{-1}\sum_{i=1}^N \left(m_i^{(k)}\right)^2 + 2N^{-1}\sum_{i=1}^N \left|1\cdot\left(m_i^{(k)} - m_i^{(k-1)}\right)\right|. \tag{2.13}$$

The second term on the r.h.s. is bounded by

$$2N^{-1/2}\left[\sum_{i=1}^N \left(m_i^{(k)} - m_i^{(k-1)}\right)^2\right]^{1/2} \tag{2.14}$$

by the Cauchy-Schwarz inequality and thus converges to 0 in probability as $N\to\infty$ followed by $k\to\infty$ by (2.2). The first term on the r.h.s. of (2.13) equals q_N and thus converges to q in probability as $N\to\infty$ followed by $k\to\infty$. From (1.2), we obtain

$$q = \mathsf{E}\tanh^2\left(h + \beta\sqrt{q}Z\right) \le h^2 + \beta^2 q\,, \tag{2.15}$$

and

$$0 \le q \le \frac{h^2}{1-\beta^2}\,, \tag{2.16}$$

for $\beta\in(0,1)$, hence $h\to 0$ implies $q\to 0$.

From the above, it follows that $\mu^{(k)}$ and $\hat{\mu}$ converge in probability to the same vague limit μ as $N\to\infty$ followed by $k\to\infty$ and $h\to 0$. For $h=0$ and $\beta\in(\sqrt{2}-1,1)$, we have $\mu(-\infty,-1)>0$ a.s. as a consequence of the first part of the proof. The assertion now follows from the vague convergence in probability of $\mu^{(k)}$ to μ. □

2.3 Musing on low temperature

Given the above, one may hope that the two-step procedure in Bolthausen's algorithm bypasses repulsiveness of TAP equations also in low temperature, but the following (non-rigorous) numerical observation, run on the High Performance Computer Elwetritsch, shows that this is hardly the case: in low temperature, 2SteB becomes so sensitive to the initialization that it is eventually hopeless at finding stable fixed points. On the other hand, a simple *reformulation* of the TAP fixpoint leads to an algorithm (out of many) seemingly overcoming this difficulty. Precisely, for $\varepsilon\in\mathbb{R}$ and $i=1\ldots N$ we set

$$m_i^{(k+1)} = \varepsilon m_i^{(k)} + (1-\varepsilon)\tanh\left(h + \frac{\beta}{\sqrt{N}}\sum_{j:\,j\neq i} g_{ij} m_j^{(k)} - \beta^2(1-q_N)m_i^{(k)}\right),\ k\in\mathbb{N}. \tag{2.17}$$

We refer to this algorithm[3] as ε-Banach: the idea behind the"ε-splitting" is to mitigate the impact of large negative Jacobian-eigenvalues. We emphasize that: *i)* we consider

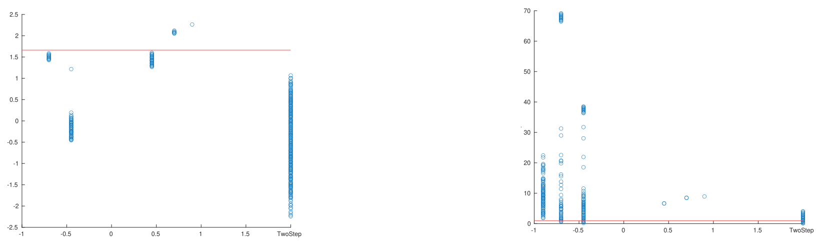
[3] This scheme is well-known in the numerical literature: it has been implemented e.g. by Aspelmeier et. al [4] to probe marginal stability of TAP solutions "at the edge of chaos".

the finite-N Onsager reaction term[4] $q_N := N^{-1}\sum_{i=1}^N {m_j^{(k)}}^2$, and *ii)* Iterations are classical: unlike (2.1), no time-delay appears in Onsager's correction. Given our limited theoretical understanding, effective ε-choices can only be found empirically. We calibrate by appealing to the *TAP free energy* (TAP FE), which maps $\boldsymbol{m} \in [-1,1]^N$ to

$$N f_{\mathrm{TAP}}(\boldsymbol{m}) \equiv \frac{\beta}{\sqrt{N}} \sum_{i<j}^{N} g_{ij} m_i m_j + h \sum_{i\le N} m_i + \frac{\beta^2}{4N} \sum_{i,j=1}^{N} (1-m_i^2)(1-m_j^2) - \sum_{i\le N} I(m_i), \tag{2.18}$$

where $I(x) \equiv \frac{1+x}{2}\log(1+x) + \frac{1-x}{2}\log(1-x)$. For an approximate solution to be physically relevant, its TAP FE should coincide[5] with the Parisi FE [13]. Critical points of the TAP FE are solutions of TAP equations: in our simulations we have computed the TAP FE of the fixed points found by both 2SteB and ε-Banach for several values of ε. This is no simple task, for multiple reasons. First, the choice of the system's size is a priori not clear: *we have chosen this to be* $N = 25$. This might look at first sight unreasonably small, but numerical evidence rejects the objection. In low temperature, the issue of initialization becomes salient, and this is oddly related to the unknown criteria for the validity of the TAP-Plefka expansions (which lead to the TAP FE). Indeed, the only criterion which seems to be unanimously accepted is Plefka's criterion, see [14],

$$\text{Plefka}\left(\boldsymbol{m}^{(k)}\right) \equiv \frac{\beta^2}{N}\sum_{i=1}^{N}\left(1-{m_i^{(k)}}^2\right)^2 \le 1,\ \forall k. \tag{2.19}$$



(a) TAP FE (y-axis) of all iterations landing inside the hypercube, the ε values are on the x-axis except for the rightmost line of blue dots which corresponds to 2SteB. The red line is at the Parisi FE ≈ 1.66 (within the 2RSB approximation).

(b) Plefka-values (y-axis) of all iterations, the ε values are on the x-axis except for the rightmost line of blue dots which corresponds to 2SteB. The large values (Plefka $\left(\boldsymbol{m}^{(k)}\right) \gg 1$) correspond to (unviable) iterates falling out of the hypercube. The red line is at $y = 1$.

Figure 2: ε-Banach vs. 2SteB: 1000 uniformly chosen initializations, k=1000 iterations each, one realization of disorder, $\beta = 3$, $h = 0.5$. One clearly evinces that 2SteB comes, in low temperature, to a stall: it doesn't even come close to a reasonable TAP FE (Figure a). For ε-Banach, two choices lead to reasonable TAP FEs: positive $\varepsilon = 0.5$ yields solutions violating Plefka's criterion (Figure b); only negative $\varepsilon \approx -0.7$ lead to viable solutions.

We thus start the algorithm near the *corners*: $\boldsymbol{m}^{(0)}$ is drawn uniformly in the subset of the hypercube where coordinates satisfy $m_\cdot^{(0)} \in [0.99, 1] \cup [-1, -0.99]$. Figure 2 compares TAP FE and Plefka-values for ε-Banach and 2SteB. Our findings come with no rigorous numerical analysis, but provide a cautionary tale when searching for TAP-solutions via fixpoints: *the way TAP-equations are written might play a bigger role than expected.*

[4]Analogously for 2SteB: the approximation (1.2) is of course wrong in low temperature.

[5]The low temperature SK-model allegedly requires ∞-many replica symmetry breakings (RSB). We use the Parisi FE obtained from a 2RSB approximation as the numerical error is mostly irrelevant [12].

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