On the Gardner formula for the perceptron

Erwin Bolthausen, University of Zurich,

joint with Shuta Nakaijma, Kyoto University

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Consider M independent, uniformly distributed, half-spaces H_k, with $0 \in \partial H_k$. How many $\sigma \in \{-1,1\}^N$ are in $\bigcap_{k=1}^M H_k$? Take $M = \alpha N$, and define

$$f(\alpha) := \lim_{N\to\infty} \frac{1}{N} \log \# \left[\{-1,1\}^N \cap \bigcap_{k=1}^{\alpha N} H_k \right].$$

Gardner's formula, first derived (non-rigorously) by Gardner-Derrida:

Theorem (Gardner-Derrida, Mézard, Talagrand). *If α is small enough, then*

$$f(\alpha) = \log 2 - \frac{\alpha r}{2}(1-q) + E_Z \log\cosh\left(\sqrt{\alpha r} Z\right) + \alpha E_Z \log \Phi\left(\frac{\sqrt{q} Z}{\sqrt{1-q}}\right),$$

where Z is a standard Gaussian, Φ the Gaussian distribution function, and $r = r(\alpha)$ and $q = q(\alpha)$ solve

$$q = E\,\mathrm{th}^2\left(\sqrt{\alpha r} Z\right),\ r = E\psi_q^2(\sqrt{q} Z),\ \psi_q(x) := \frac{1}{\sqrt{1-q}} \frac{\varphi\left(x/\sqrt{1-q}\right)}{\Phi\left(x/\sqrt{1-q}\right)}.$$

φ the standard normal density.

Remark: Gardner-Derrida claim (based on replica computation) that the formula is correct up to

$$\alpha^* := \sup\{\alpha > 0 : f(\alpha) > 0\} < 1,$$

and that $\# = 0$ a.s. for $\alpha > \alpha^*$.

Remark: For *no* $\alpha > 0$ is it true that $f(\alpha)$ equals

$$f_{\text{ann}}(\alpha) := \lim_{N\to\infty} \frac{1}{N} \log \mathbb{E}\# \left[\{-1,1\}^N \cap \bigcap_{k=1}^{\alpha N} H_k \right] = (1-\alpha)\log 2.$$

Talagrand: Consider $u : \mathbb{R} \to [-\infty, \infty)$, with some upper bound (square increase is not allowed), and with i.i.d. standard Gaussians $(J_{ik})_{i \le N,\ k \le M}$

$$Z_{N,\alpha,u} := \sum_{\sigma \in \{-1,1\}^N} \exp\left[\sum_{k=1}^{\alpha N} u\left(\sum_{i=1}^{N} \sigma_i \frac{J_{ik}}{\sqrt{N}} \right) \right].$$

The half-space case is $u(x) := -\infty 1_{x<0}$. For general u, one has

$$\psi_q(x) := \frac{1}{\sqrt{1-q}} \frac{E\left(Z \exp\left[u\left(x+\sqrt{1-q}Z\right)\right]\right)}{E\left(\exp\left[u\left(x+\sqrt{1-q}Z\right)\right]\right)},$$

and the replica symmetric formula for $f(\alpha, u) := \lim_{N\to\infty} N^{-1} \log Z_{N,\alpha,u}$ is

$$\begin{aligned} f(\alpha, u) &= \log 2 - \frac{\alpha r}{2}(1-q) + E_Z \log\cosh\left(\sqrt{\alpha r}Z\right) \\ &\quad + \alpha E_Z \log E_{Z'} \exp\left[u\left(\sqrt{q}Z + \sqrt{1-q}Z'\right)\right]. \end{aligned}$$

again with $q = E\,\mathrm{th}^2\left(\sqrt{\alpha r}Z\right),\ r = E\psi_q^2\left(\sqrt{q}Z\right)$. Talagrand first proves the result for smooth u by a perturbative method, and then uses a complicated approximation for $u = -\infty 1_{x<0}$.
Remark: ψ_q is smooth for non-smooth u.

The problem comes up in connection with the memory capacity in neural nets, in particular the **perceptron,** but it is also related to other models, e.g. in compressed sensing.

Standard second moment method: one tries to prove, for a sequence $\{Z_N\}$ of random partition functions, that

$$\mathbb{E}Z_N^2 \leq \mathsf{const} \times (\mathbb{E}Z_N)^2$$

in which case one obtains, with a self-averaging property

$$\lim_{N\to\infty} \frac{1}{N} \log Z_N = f_{\mathsf{ann}} := \lim_{N\to\infty} \frac{1}{N} \log \mathbb{E}Z_N$$

which evidently cannot work in our case. Also for the **Sherrington-Kirkpatrick model** with *non-vanishing* external field:

$$Z_{N,\beta,h} := \sum_{\boldsymbol{\sigma}} 2^{-N} \exp\left[\frac{\beta}{\sqrt{2N}} \sum\nolimits_{1\leq i<j\leq N} J_{ij}\sigma_i\sigma_j + h \sum\nolimits_{i=1}^{N} \sigma_i\right], \ h \neq 0,$$

For *no* $\beta > 0$, $h \neq 0$, one has $f = f_{\mathsf{ann}}$.

Morita argument: find a "proper" sequence of σ-fields $\mathcal{G}_N$ and prove

$$\mathbb{E}\left(Z_N^2 \middle| \mathcal{G}_N\right) \leq C_N \mathbb{E}\left(Z_N \middle| \mathcal{G}_N\right)^2 ,$$

$C_N = \mathrm{e}^{o(N)}$, and $\lim_{N\to\infty} N^{-1} \log \mathbb{E}\left(Z_N \middle| \mathcal{G}_N\right) = f$. Then $f = \lim_{N\to\infty} N^{-1} \log Z_N$.
For the SK and the perceptron, take $\mathcal{G}_N = \sigma\left(m_i : i \leq N\right)$, where $m_i := \langle \sigma_i \rangle$.
Thouless-Anderson-Palmer equations. For SK:

$$m_i = \mathrm{th}\left(h + \beta \sum_{j=1}^{N} \frac{J_{ij}}{\sqrt{N}} m_j \underbrace{- \beta^2 \left(1 - N^{-1} \sum_j m_j^2\right) m_i}_{\text{Onsager correction}}\right).$$

Heuristic derivation by belief propagation (at high temperature)

$$m_i = \mathrm{th}\left(h + \beta \sum_{j=1}^{N} \frac{J_{ij}}{\sqrt{N}} m_j^{\text{cut } i}\right), \ \frac{1}{N} \sum_i m_i^2 \approx q, \ q = E_Z \, \mathrm{th}^2\left(h + \beta \sqrt{q} Z\right)$$

For the perceptron, TAP equations were first derived by Mézard: Best also by belief propagation (see Mézard 2017 for the Hopfield model). Formally, one relates the m_i to

$$n_k := \left\langle u'\left(S_k\right)\right\rangle,\ S_k := \sum_{i=1}^{N} \sigma_i \frac{J_{ik}}{\sqrt{N}}$$

The equations are

$$\begin{aligned} m_i &= \mathrm{th}\left(N^{-1/2} \sum_{k=1}^{M=\alpha N} J_{ik} n_k - \alpha E_Z \psi_q'\left(\sqrt{q} Z\right) m_i\right) \\ n_k &= \psi_q\left(N^{-1/2} \sum_{i=1}^{N} m_i J_{ik} - (1-q)\, n_k\right), \end{aligned}$$

where q comes from the fixed point equation above.

For $q \in (0,1)$, ψ_q is smooth regardless if u is: The equations make sense for non-smooth u.

The proper way to construct directly TAP solutions (in high temperature) for SK was done in my 2015 CMP paper. The method can be adapted for the perceptron: joint work with **Shuta Nakaijma**, Kyoto University.

Take $m_i^{[0]} := 0,\ m_i^{[1]} := \sqrt{q},\ n_k^{[0]} = 0,\ n_k^{[1]} := \sqrt{r}$, and

$$\begin{aligned} m_i^{[t+1]} &= \mathrm{th}\left(N^{-1/2}\sum\nolimits_{k=1}^{\alpha N} J_{ik} n_k^{[t]} - m_i^{[t-1]} \alpha E \psi_q'\left(\sqrt{q}Z\right)\right), \\ n_k^{[t+1]} &= \psi_q\left(N^{-1/2}\sum\nolimits_{i=1}^{N} m_i^{[t]} J_{ik} - n_k^{[t-1]}(1-q)\right). \end{aligned}$$

The time shift for the Onsager corrections were "observed" before my paper by Donoho & Montanari for compressed sensing algorithms, and they checked the effectivity numerically.

Theorem *Assume* $\sup_x \left|\psi_q'(x)\right| < \infty$ *(which is satisfied for* $u = -\infty 1_{x<0}$*), and that* $q = E\,\mathrm{th}^2(\sqrt{\alpha r}Z)$, $r = E\psi_q^2\left(\sqrt{q}Z\right)$ *has a unique solution (which is easy for small* α*, and may be correct for all* α*). Then*

$$\begin{aligned} \lim_{s,t\to\infty} \limsup_{N\to\infty} \mathbb{E}\frac{1}{N}\sum_i \left(m_i^{[s]} - m_i^{[t]}\right)^2 &= 0, \\ \lim_{s,t\to\infty} \limsup_{M\to\infty} \mathbb{E}\frac{1}{M}\sum_k \left(n_k^{[s]} - n_k^{[t]}\right)^2 &= 0 \end{aligned}$$

under a condition resembling the de Almeida–Thouless condition for SK:

$$\alpha E\frac{1}{\cosh^4(\sqrt{\alpha r}Z)} E\left[\psi_q'(\sqrt{q}Z)\right]^2 \leq 1.$$

The dependence of the iterates $m^{[t]}$ and $n^{[t]}$ on $\left(J_{ij}\right)$ can precisely be described (which would not be the case without the time shift of the Onsager correction).

For fixed t, and $N \to \infty$, there is a representation

$$
\begin{aligned}
m_i^{[t+1]} &\approx \text{th}\left(N^{-1/2}\sum_{k=1}^{\alpha N} J_{ik}^{[t]} n_k^{[t]} + \gamma_1 \xi_i^{[1]} + \cdots + \gamma_{k-1}\xi_i^{[t-1]}\right), \\
n_k^{[t+1]} &\approx \psi_q\left(N^{-1/2}\sum_{i=1}^{N} J_{ik}^{[t]} m_i^{[t]} + \delta_1 \eta_k^{[1]} + \cdots + \delta_{k-1}\eta_k^{[t-1]}\right),
\end{aligned}
$$

with inductively defined $\gamma_i, \delta_i \in \mathbb{R}$, random variables $\xi_i^{[s]}, \eta_i^{[s]}$ which asymptotically ($N \to \infty$) are Gaussian, and matrices $\left(J_{ik}^{[t]}\right)_{i \leq N,\ k \leq \alpha N}$ that are *conditionally* Gaussian given $\mathcal{G}_{t-1} := \sigma\left(\xi^{[s]}, \eta^{[s]} : s \leq t-1\right)$.

They have the following covariances:

$$\mathbb{E}\left(J_{ij}^{[t]} J_{k\ell}^{[t]} \middle| \mathcal{G}_{t-1} \right) = \left(\delta_{ik} - \alpha_{ik}^{[t-1]} \right) \left(\delta_{j\ell} - \beta_{j\ell}^{[t-1]} \right),$$

with

$$\alpha_{ij}^{[m]} := \frac{1}{N} \sum_{s=1}^{m} \phi_i^{[s]} \phi_j^{[s]}, \ \beta_{ij}^{[m]} := \frac{1}{M} \sum_{s=1}^{m} \psi_i^{[s]} \psi_j^{[s]},$$

where $\phi^{[s]} \in \mathbb{R}^N$ are from the $m^{[s]}$ by Gram-Schmidt, and $\psi^{[s]}$ the same in $\mathbb{R}^M$. The $J^{[t]}$ are obtained from J with a series of rank one corrections:

$$J_{ij}^{[t]} = J_{ij} - \sum_{s=1}^{t-1} \rho_{ij}^{[s]}, \ \rho_{ij}^{[s]} := \frac{\xi_i^{[s]} \psi_j^{[s]}}{\sqrt{N}} + \frac{\phi_i^{[s]} \eta_j^{[s]}}{\sqrt{N}} + \text{correction}.$$

Two crucial points:

- The AT-condition is satisfied iff the first parts $N^{-1/2}\sum_{k=1}^{\alpha N} J_{ik}^{[t]} n_k^{[t]}$, $N^{-1/2}\sum_{i=1}^{N} m_i^{[t]} J_{ik}$, disappear asymptotically ($N \to \infty$ first, and then $t \to \infty$). This is due to combined properties of $J^{[t]}$ and $n^{[t]}, m^{[t]}$. From this one derives the above theorem.

- The $J^{[t]}$ stays "close" to J, as $N \to \infty$, for instance if $x \in \mathbb{R}^N$ then the vector $Y := xJ^{[t]}$ has a covariance matrix of rank $N - t + 1$.

The key idea for the free energy is to tilt the coin tossing measure $p_0(\sigma) := 2^{-N}$, to

$$p^{[t+1]}(\sigma) = \prod_{i=1}^{N} p_i^{[t+1]}(\sigma_i), \; p_i^{[t+1]}(\sigma_i) = \frac{1}{2}\frac{\mathrm{e}^{h_i^{[t+1]}\sigma_i}}{\cosh\left(h_i^{[t+1]}\right)}, \; m_i^{[t+1]} = \mathrm{th}\left(h_i^{[t+1]}\right),$$

and to write

$$\sum_{\sigma} 2^{-N} \exp\left[\sum\nolimits_k u(S_k)\right] = \prod_i \cosh\left(h_i^{[t+1]}\right) Z'_N,$$

$$Z'_N \quad := \sum\nolimits_{\sigma} p^{[t+1]}(\sigma) \exp\left[\sum\nolimits_k u(S_k) - \sum\nolimits_i h_i^{[t+1]} \sigma_i\right]$$

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \log\cosh\left(h_i^{[t+1]}\right) = E_Z \log\cosh\left(\sqrt{\alpha r} Z\right)$$

a.s. and in L_1. $p^{[t+1]}(\sigma)$ is $\mathcal{G}_t$-m.b., and one would like to prove that as $N \to \infty,\ t \to \infty$

$$N^{-1} \log \mathbb{E}_t Z'_N = N^{-1} \log \sum\nolimits_{\sigma} p^{[t+1]}(\sigma)\, \mathbb{E}_t \exp\left[\sum\nolimits_k u(S_k) - \sum\nolimits_i h_i^{[t+1]} \sigma_i\right]$$

$$\to -\frac{\alpha r}{2}(1-q) + \alpha E_Z \log E_{Z'} \exp\left[u\left(\sqrt{q} Z + \sqrt{1-q} Z'\right)\right],$$

plus an estimate of the second moment. $\mathbb{E}_t := \mathbb{E}\left(\cdot \mid \mathcal{G}_t\right)$.

The SK is simpler (and done): After a simple computation (and some approximations), one gets with $\hat{\sigma}_i = \sigma_i - m_i^{[t+1]}$, and with $\langle x, y \rangle := N^{-1} \sum_{i=1}^N x_i y_i$

$$\mathbb{E}_t Z'_N = \exp\left[N \frac{\beta^2 (1-q)^2}{4}\right]$$
$$\times \sum_\sigma p^{[t+1]}(\sigma)\, \mathbb{E}_t \exp\left[\frac{\beta\sqrt{N}}{\sqrt{2}} \langle \hat{\sigma}, J\hat{\sigma} \rangle - \frac{\beta^2 N \|\hat{\sigma}\|^4}{4} + \beta^2 N \left\langle m^{[t+1]}, \hat{\sigma} \right\rangle^2\right],$$

with q satisfying $q = E\, \mathrm{th}^2\left(h + \beta\sqrt{q} Z\right)$. If $\sum_\sigma \cdots = \mathrm{e}^{o(N)}$, we are done (for the first moment).

Assume *wrongly* that J_{ij}, under $\mathbb{E}_t$ are i.i.d. and independent of $m_i^{[t+1]}$, then

$$\sum_\sigma \cdots = \sum_\sigma p^{[t+1]}(\sigma) \exp\left[\beta^2 N \left\langle m^{[t+1]}, \hat{\sigma} \right\rangle^2\right]$$

and we are left with a Curie-Weiss type term, which is $\mathrm{e}^{o(N)}$ below AT. A similar straightforward (but wrong!) argument gives the Gardner-formula in the perceptron.

For SK: Replace J by $J^{[t+1]} + \sum$of rank one corrections, which essentially adds in the Hamiltonian

$$\beta \sum_{s=1}^{t} N \left\langle \hat{\sigma}, \xi^{[s]} \right\rangle \left\langle \hat{\sigma}, \phi^{[s]} \right\rangle$$

which is still of Curie-Weiss type. We still have to evaluate

$$\mathbb{E}_t \exp \left[\frac{\beta\sqrt{N}}{\sqrt{2}} \left\langle \hat{\sigma}, J^{[t+1]} \hat{\sigma} \right\rangle - \frac{\beta^2 N \left\| \hat{\sigma} \right\|^4}{4} \right].$$

$J^{[t+1]}$ is conditionally Gaussian given $\mathcal{G}_t$, leading to no additional trouble, *except* one has infinitely many Curie-Weiss terms in the $t \to \infty$ limit, and one has to check that they are not distroying the picture

This step is however rather delicate for the perceptron, as the Gaussians are inside the function u, which may even be discontinuous e.g. $u(x) = -\infty 1_{x<0}$.

The second conditional moment is similar, with additional Curie-Weiss terms. The result (for SK) is

$$\begin{aligned} \lim_{t\to\infty} \limsup_{N\to\infty} \mathbb{E}\left|\frac{1}{N}\log \mathbb{E}_t Z_N - \mathsf{RS}\left(\beta, h\right)\right| &= 0, \\ \lim_{t\to\infty} \limsup_{N\to\infty} \mathbb{E}\left|\frac{1}{N}\log \mathbb{E}_t Z_N^2 - 2\,\mathsf{RS}\left(\beta, h\right)\right| &= 0, \end{aligned}$$

where

$$\mathsf{RS}\left(\beta, h\right) = E_Z \log\cosh\left(h + \beta\sqrt{q}Z\right) + \frac{\beta^2\left(1-q\right)^2}{4},$$

which proves

$$\lim_{N\to\infty} \frac{1}{N}\mathbb{E}\log Z_N = \mathsf{RS}\left(\beta, h\right).$$

Remarks:

a) "In principle", the method is non-perturbative. The only place where we have to rely on "small β" are the Curie-Weiss computations for which the correct critical value is a bit delicate. For the first moment, I think it is OK up to AT, but certainly not for the second. For the perceptron, we in addition need the uniqueness of the fixed point equation for (q, r).

b) The method seems to be applicable in cases where there are TAP type equations.

c) A somewhat similar idea is used in a paper by Fan, Mei, and Montanari (Aug 2018).

d) Similar TAP-type structures appear in connection with compressed sensing, and variants of the above representations have been obtained in this context by Bayati, Donoho, Montanari, Lelarge, and others.

e) It is suggestive to conjecture that the Curie-Weiss terms describe the finite size corrections.

d) The main shortcoming is that the method is for the moment restricted to the replica symmetric region. For diluted models, there is a non-rigorous approach by Mézard, Parisi, Montanari for the BP equations in the 1RSB case, but I don't now if it could be adapted to TAP equations (even non-rigorously).

Happy (After)Birthday, Anton!