Inference from correlated patterns: a unified theory for perceptron learning and linear vector channels

Yoshiyuki Kabashima
Department of Computational Intelligence and Systems Science, Tokyo Institute of Technology, Yokohama 226-8502, Japan
E-mail: kaba@dis.titech.ac.jp

Abstract. A framework to analyze inference performance in densely connected single-layer feed-forward networks is developed for situations where a given data set is composed of correlated patterns. The framework is based on the assumption that the left and right singular value bases of the given pattern matrix are generated independently and uniformly from Haar measures. This assumption makes it possible to characterize the objective system by a single function of two variables which is determined by the eigenvalue spectrum of the cross-correlation matrix of the pattern matrix. Links to existing methods for analysis of perceptron learning and Gaussian linear vector channels and an application to a simple but nontrivial problem are also shown.

1. Introduction
Inference from data is one of the most significant problems in information science, and perceptrons (or single-layer feed-forward networks) are often included in widely-used devices for solution of this problem. In the general scenario, for a given \( N \) dimensional input pattern \( \mathbf{x} = (x_1, x_2, \ldots, x_N)^T \), such a network returns an output \( y \), which may be a continuous/discrete single/multidimensional variable, following a conditional probability distribution

\[
P(y|\mathbf{x}; \mathbf{w}) = P(y|\Delta),
\]

where \( \mathbf{T} \) denotes the matrix transpose, \( \mathbf{w} = (w_1, w_2, \ldots, w_N)^T \) denotes the weight parameter of the perceptron and \( \Delta = N^{-1/2} \mathbf{w} \cdot \mathbf{x} \). The scale factor \( N^{-1/2} \) is introduced to ensure that the components of \( \mathbf{w} \) and \( \mathbf{x} \) are typically of \( O(1) \) as the limit of \( N \to \infty \). Given a data set \( \xi^p = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_p, y_p)\} \), the Bayes formula

\[
P(\mathbf{w}|\xi^p) = \frac{1}{Z_p(\xi^p)} P(\mathbf{w}) \prod_{\mu=1}^p P(y_{\mu}|\Delta_{\mu}),
\]

provides us with a useful basis for constructing the optimal inference, which may for example involve estimation of the parameter \( \mathbf{w} \), or prediction of outputs for novel input patterns. Here \( P(\mathbf{w}) \) is a certain prior distribution of \( \mathbf{w} \), \( \Delta_{\mu} = N^{-1/2} \mathbf{w} \cdot \mathbf{x}_{\mu} \) (\( \mu = 1, 2, \ldots, p \)) and the normalization factor \( Z_p(\xi^p) = \text{Tr}_\mathbf{w} P(\mathbf{w}) \prod_{\mu=1}^p P(y_{\mu}|\Delta_{\mu}) \) serves as a partition function, where \( \text{Tr}_\mathbf{w} \) denotes summation (or integration) over all possible states of \( \mathbf{w} \).

In general, equation (1) can be regarded as the canonical distribution of a virtual spin system which is subject to random interactions. This similarity has motivated cross-disciplinary research across the fields of statistical mechanics and neural information processing over the last two decades, which has led to the discovery of various complex behaviors in the learning processes of...
neural networks [1, 2, 3] and to the development of families of advanced mean field approximation algorithms that practically overcome the intrinsic computational difficulties underlying inference in large networks [4, 5].

More recently, inference in the style of equation (1) is also being researched actively in another context: namely, in the study of linear vector channels for wireless communication. In this context, multiple information symbols denoted by $\mathbf{w}$ are simultaneously transmitted through a single channel, linearly transformed into $\Delta_\mu = N^{-1/2}x_\mu \cdot \mathbf{w}$ ($\mu = 1, 2, \ldots, p$). At the receiver's terminal, the transmitted symbols $\mathbf{w}$ have to be estimated from the received signals $y_\mu$ ($\mu = 1, 2, \ldots, p$). Under the assumption that the channel and the prior distribution of information symbols are modeled as $\prod_{\mu=1}^p P(y_\mu | \Delta_\mu)$ and $P(\mathbf{w})$, respectively, equation (1) allows the optimal demodulation scheme. The similarity between problems of inference and disordered spin systems again serves to potentiate nontrivial performance analysis [6, 7, 8, 9, 10, 11, 12, 13] and development of advanced approximate demodulation algorithms [14, 15, 16, 17, 18] for large systems.

Although statistical mechanical schemes have been applied successfully to various inference problems of the form of equation (1) in such ways, there still remain several research directions to explore. Investigation of inference from correlated patterns is a typical example of such a problem. For theoretical simplicity, most existing research on perceptron learning is based on the assumption that the input vectors are independently generated from an isotropic distribution [1, 2, 3]. However, it is obvious that real world data is usually somewhat biased and correlated across components, which makes it difficult to utilize the developed schemes directly for data analysis beyond a conceptual level. Exploration of correlated patterns is also important in the study of linear vector channels because the matrix entries of the linear transformation are generally correlated with each other due to spatial proximity of antennas and for optimizing communication performance [19, 20]. Recently, the author and his colleagues have developed a framework to handle such situations based on a formula of random matrix theory [21, 22]. However, the scheme we have developed is still not fully satisfactory because it is applicable only to Gaussian channels. In order to deal with more general situations, further development is required.

The purpose of this article is to provide such a development. More precisely, we will develop a framework to analyze inference offered by equation (1) when entries of the pattern matrix

$$X = N^{-1/2}(x_1, x_2, \ldots, x_p)^T,$$

(2)

are correlated. A similar direction has already been followed by Opper and Winther [23, 24, 25]. However, their formalism, developed for densely connected networks of two-body interactions, is highly general, and therefore properties that hold specifically for models satisfying equation (1) are not fully utilized. Hence we develop here a specific formalism for analyzing inference problems expressed by means of equation (1).

This article is organized as follows. In section 2, models that we will investigate are introduced. For characterizing correlated patterns, we assume that the pattern matrix (2) is randomly generated under the constraint that singular values of the matrix obey a given distribution. Section 3 is the main part of this article, in which two analytical schemes are developed. One takes as its basis the replica method [26], which makes it possible to assess the typical inference performance of the objective system by averaging the pattern matrix $X$ with respect to an assumed distribution. The other is developed for approximately evaluating the average of $\mathbf{w}$ with respect to equation (1) for a given specific $X$ (or $\xi^p$), which corresponds to the Thouless-Anderson-Palmer approach [27] in spin glass research. It is shown that a two-variable function, which we denote by $F(x, y)$ and which is determined by the eigenvalue spectrum of the cross-correlation matrix $X^T X$ and the pattern ratio $\alpha = p/N$, plays an important role in both schemes. Links to existing methods of analysis of the schemes that we develop are indicated.
in section 5 in conjunction with an application to a simple example problem. The final section contains a summary.

2. Model definition
An expression of the singular value decomposition

$$X = U^T D V,$$  

(3)

of the pattern matrix $X$ is the basis of our framework, where $D = \text{diag}(d_k)$ is a $p \times N$ diagonal matrix, and $U$ and $V$ are $p \times p$ and $N \times N$ orthogonal matrices, respectively. Linear algebra guarantees that an arbitrary $p \times N$ matrix $X$ can be decomposed according to equation (3). The singular values of $X$, $d_k$ ($k = 1, 2, \ldots, \min(p, N)$), are linked to eigenvalues of the cross correlation $X^T X$, $\lambda_k$ ($k = 1, 2, \ldots, N$), as $\lambda_k = d_k^2$ ($k = 1, 2, \ldots, \min(p, N)$) and 0 otherwise, where $\min(p, N)$ denotes the lesser value of $p$ and $N$. In order to handle correlations in $X$ analytically, we assume that the orthogonal matrices $U$ and $V$ are uniformly and independently generated from the Haar measures of $p \times p$ and $N \times N$ orthogonal matrices, respectively, and that the empirical eigenvalue spectrum of $X^T X$, $N^{-1} \sum_{k=1}^N \delta(\lambda - \lambda_k) = (1 - \min(p, N)/N)\delta(\lambda) + N^{-1} \sum_{k=1}^{\min(p,N)} \delta(\lambda - d_k^2)$, converges to a certain distribution $\rho(\lambda)$ as $N$ and $p$ tend to infinity with keeping $\alpha = p/N$ of the order of unity.

For generality, we assume that the outputs $y = (y_1, y_2, \ldots, y_p)^T$ for $X$ are generated from a generative model

$$Q(y|X) = \text{Tr}_{w} Q(w) \prod_{\mu=1}^p Q(y_{\mu}|\Delta_{\mu}) = Z_Q(\xi^w),$$  

(4)

where the prior and conditional probabilities of this model, $Q(w)$ and $Q(y|\Delta)$, may differ from those of the recognition model, $P(w)$ and $P(y|\Delta)$, which is used in equation (1). For a fixed data set $\xi^w = \{(x_1, y_1), (x_2, y_2), \ldots, (x_p, y_p)\} = (X, y)$, $Q(y|X) = Z_Q(\xi^w)$ serves as the partition function of the correct posterior distribution of $w$, $Q(w|\xi^w) = Q(w) \prod_{\mu=1}^p Q(y_{\mu}|\Delta_{\mu})/Z_Q(\xi^w)$. For analytical tractability, we also assume that both the prior distributions of the generative and recognition models can be factorized as $Q(w) = \prod_{i=1}^N Q(w_i)$ and $P(w) = \prod_{i=1}^N P(w_i)$, respectively.

3. Analysis
3.1. Analysis of the generative model and the $F$-function
We first analyze properties of the generative model since outputs $y$ of the data set $\xi^w$ are generated by this model following equation (4). For this purpose, we introduce an expression

$$Z_Q(\xi^w) = \text{Tr}_w \prod_{i=1}^N Q(w_i) \prod_{\mu=1}^p \left( \int d\Delta_{\mu} Q(y_{\mu}|\Delta_{\mu}) \delta(\Delta_{\mu} - N^{-1/2}w \cdot x_{\mu}) \right)$$

$$= \int \prod_{\mu=1}^p \left( \frac{du_{\mu}d\Delta_{\mu}}{2\pi} \exp[-iu_{\mu}\Delta_{\mu}] Q(y_{\mu}|\Delta_{\mu}) \right) \text{Tr}_w \prod_{i=1}^N Q(w_i) \exp[iu^T X w]$$

$$= \text{Tr}_w \prod_{\mu=1}^p \tilde{Q}_{y_{\mu}}(u_{\mu}) \prod_{i=1}^N Q(w_i) \exp[iu^T X w],$$  

(5)

where $i = \sqrt{-1}$, $u = (u_1, u_2, \ldots, u_p)^T$ and $\tilde{Q}_{y_{\mu}}(u_{\mu}) = \int d\Delta_{\mu} \exp[-iu_{\mu}\Delta_{\mu}] Q(y_{\mu}|\Delta_{\mu})/(2\pi)$. Next, we substitute equation (3) into equation (5) and take an average with respect to the orthogonal
matrices $U$ and $V$. For this evaluation, it is noteworthy that for fixed sets of dynamical variables $w$ and $u$, $\tilde{w} = Vw$ and $\tilde{u} = Uu$ behave as continuous random variables which are uniformly generated under the strict constraints

$$\frac{1}{N} |\tilde{w}|^2 = \frac{1}{N} |w|^2 = T_w, \quad (6)$$
$$\frac{1}{p} |\tilde{u}|^2 = \frac{1}{p} |u|^2 = T_u, \quad (7)$$

when $U$ and $V$ are independently and uniformly generated from the Haar measures. In the limit as $N, p \to \infty$ with keeping $\alpha = p/N O(1)$, this yields an expression

$$\frac{1}{N} \ln \left[ \exp \left[ i u^T X w \right] \right] = F(T_w, T_u), \quad (8)$$

where $\langle \cdot \rangle$ denotes averaging with respect to the Haar measures, the function $F(x, y)$ is defined as

$$F(x, y) = \operatorname{Extr}_{\Lambda_x, \Lambda_y} \left\{ -\frac{1}{2} ( \ln(\Lambda_x \Lambda_y + \lambda) )_\rho - \frac{\alpha - 1}{2} \ln \Lambda_y + \frac{\Lambda_x x^2}{2} + \frac{\alpha \Lambda_y y^2}{2} \right\}$$
$$- \frac{1}{2} \ln x - \frac{\alpha}{2} \ln y - \frac{1 + \alpha}{2}, \quad (9)$$

and $\langle \cdot \rangle_\rho$ indicates averaging with respect to the asymptotic eigenvalue spectrum of $X^T X$, $\rho(\lambda)$. $\operatorname{Extr} \{ \cdot \}$ represents extremization with respect to $\theta$, which corresponds to the saddle point assessment of a complex integral and therefore does not necessarily mean operation of minimum or maximum. Expressions analogous to equations (8) and (9) are known as the Itzykson-Zuber integral or $G$-function for ensembles of square (symmetric) matrices [28, 29, 30, 31]. These equations imply that the annealed average of equation (5) is evaluated as

$$\frac{1}{N} \ln \left[ \operatorname{Tr} y \overline{Z}_Q(x^\rho) \right] = \operatorname{Extr}_{\hat{T}_w, \hat{T}_u} \left\{ F(T_w, T_u) + A_w(T_w) + \alpha A_u(T_u) \right\}, \quad (10)$$

where

$$A_w(T_w) = \operatorname{Extr}_{\hat{T}_w} \left\{ \frac{\hat{T}_w T_w}{2} + \ln \left[ \operatorname{Tr} \hat{Q}(w) \exp \left[ -\frac{\hat{T}_w T_w}{2} w^2 \right] \right] \right\}, \quad (11)$$
$$A_u(T_u) = \operatorname{Extr}_{\hat{T}_u} \left\{ \frac{\hat{T}_u T_u}{2} + \ln \left[ \operatorname{Tr} \hat{Q}_u(u) \exp \left[ -\frac{\hat{T}_u T_u}{2} u^2 \right] \right] \right\}. \quad (12)$$

Normalization constraints $\operatorname{Tr}_y Q(y|\Delta) = 1$ guarantee that $\operatorname{Tr}_y \overline{Z}_Q(x^\rho) = 1$, which, in conjunction with equations (10), (11) and (12), implies that $T_w = \operatorname{Tr}_w w^2 Q(w)$, $T_u = 0$, $\hat{T}_w = 0$ and $\hat{T}_u = \alpha^{-1} T_u \langle \lambda \rangle_\rho$. The physical implication is that, due to the central limit theorem, $\Delta = (\Delta_1, \Delta_2, \ldots, \Delta_p)^T$ follows an isotropic Gaussian distribution

$$Q(\Delta) = \frac{1}{(2\pi T_u)^{p/2}} \exp \left[ -\frac{\Delta^2}{2 T_u} \right] = \frac{\alpha^{p/2}}{(2\pi T_w \langle \lambda \rangle_\rho)^{p/2}} \exp \left[ -\frac{\alpha \Delta^2}{2 T_w \langle \lambda \rangle_\rho} \right], \quad (13)$$

in the limit as $N, p \to \infty$, $\alpha = p/N \sim O(1)$ when $w$ is generated from $Q(w) = \prod_{i=1}^N Q(w_i)$, and $U$ and $V$ are independently and uniformly generated from the Haar measures.
3.2. Replica analysis

Now, we are ready to analyze equation (1). As $\xi^p$ is a set of predetermined random variables depending on $X$ and the generative model (5), we utilize the replica method. This means that we evaluate the $n$-th moments of the partition function $Z_P(\xi^p)$ for natural numbers $n \in \mathbb{N}$ as

$$[Z^p_\xi(\xi^p)]_{\xi^p} = \text{Tr}_{\{u^a\}} \frac{\text{Tr}_y Q(y|X) Z^p_\xi(\xi^p)}{\text{Tr}_y Z_Q(\xi^p) Z^p_\xi(\xi^p)}$$

$$= \text{Tr}_{\{u^a\}} \prod_{\mu=1}^p \left( \text{Tr}_{y_\mu} \hat{Q}_{y_\mu}(u^0_\mu) \prod_{a=1}^n \hat{P}_{y_\mu}(u^a_\mu) \right) \times \prod_{i=1}^N \left( Q(u^0_i) \prod_{a=1}^n P(u^a_i) \right)$$

$$\times \exp \left[ i \sum_{a=0}^n (u^a)^T X w^a \right], \quad (14)$$

and assess the quenched average of free energy with respect to the data set $\xi^p$ as $N^{-1} \ln Z_P(\xi^p) |_{\xi^p} = \lim_{n \to 0} N^{-1} \ln \left[ [Z^p_\xi(\xi^p)]_{\xi^p} \right]$, analytically continuing expressions obtained for equation (14) from $n \in \mathbb{N}$ to real numbers $n \in \mathbb{R}$. Here, $[\cdots]_{\xi^p} = \text{Tr}_y \hat{Q}(y|X)(\cdots) = \text{Tr}_y Z_Q(\xi^p)(\cdots)$ represents the average with respect to the data set $\xi^p$, $\hat{P}_{y_\mu}(u_\mu) = \int d\Delta_\mu \exp[-i y_\mu \Delta_\mu] P(y_\mu|\Delta_\mu)/(2\pi)$. \{w^a\} and \{u^a\} represent sets of dynamical variables $w^b, w^1, \ldots, w^n$ and $u^1, u^1, \ldots, u^n$, respectively, where the replica indices $0$ and $1, 2, \ldots, n$ denote the generative and $n$ replicas of recognition models, respectively.

For this procedure, a note similar to that for the evaluation of equation (8) is useful. Namely, for fixed sets of dynamical variables $\{u^a\}$ and $\{w^a\}$, $\tilde{u}^a = U u^a$ and $\tilde{w}^a = V w^a$ behave as continuous random variables which satisfy strict constraints

$$\frac{1}{N} \tilde{w}^a \cdot \tilde{w}^b = \frac{1}{N} w^a \cdot w^b = q^{ab},$$

$$\frac{1}{p} \tilde{u}^a \cdot \tilde{u}^b = \frac{1}{p} u^a \cdot u^b = q^{ab}, \quad (15)$$

$a, b = 0, 1, \ldots, n$ when $U$ and $V$ are independently and uniformly generated from the Haar measures. This indicates that equation (14) can be evaluated by the saddle point method with respect to sets of macroscopic parameters $\mathcal{Q}_w = (q^{ab}_w)$ and $\mathcal{Q}_u = (q^{ab}_u)$ in the limit as $N, p \to \infty$, $\alpha = p/N \sim O(1)$. In addition, intrinsic permutation symmetry among replicas indicates that it is natural to assume that $(n+1) \times (n+1)$ matrices $\mathcal{Q}_w$ and $\mathcal{Q}_u$ are of the form

$$\mathcal{Q}_w = \begin{pmatrix} T_w & m_w & m_w & \ldots & m_w \\
 m_w & \chi + q_w & q_w & \ldots & q_w \\
 m_w & q_w & \chi + q_w & \ldots & q_w \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 m_w & q_w & q_w & \ldots & \chi + q_w \\
 \sqrt{nm_w} & \sqrt{nm_w} & \chi + q_w & 0 & \ldots & 0 \\
 \sqrt{nm_w} & \chi + q_w & 0 & \ldots & 0 \\
 0 & 0 & \chi_w & 0 & \ldots & 0 \\
 0 & 0 & 0 & \chi_w & \ldots & 0 \\
 \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
 0 & 0 & 0 & 0 & \chi_w & \ldots & 0 \end{pmatrix} \times E^T,$$  

$$\mathcal{Q}_u = \begin{pmatrix} T_u & m_u & m_u & \ldots & m_u \\
 m_u & q_u & q_u & \ldots & q_u \\
 m_u & q_u & q_u & \ldots & q_u \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 m_u & q_u & q_u & \ldots & \chi + q_u \\
 \sqrt{nm_u} & \sqrt{nm_u} & \chi + q_u & 0 & \ldots & 0 \\
 \sqrt{nm_u} & \chi + q_u & 0 & \ldots & 0 \\
 0 & 0 & \chi_u & 0 & \ldots & 0 \\
 0 & 0 & 0 & \chi_u & \ldots & 0 \\
 \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
 0 & 0 & 0 & 0 & \chi_u & \ldots & 0 \end{pmatrix} \times E^T,$$ \quad (17)
and

\[
Q_u = \begin{pmatrix}
T_u & -m_u & -m_u & \ldots & -m_u \\
-m_u & \chi_u - q_u & -q_u & \ldots & -q_u \\
-m_u & -q_u & \chi_u - q_u & \ldots & -q_u \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-m_u & -q_u & -q_u & \ldots & \chi_u - q_u \\
\end{pmatrix}
= E \times
\begin{pmatrix}
T_u & -\sqrt{\pi m_u} & 0 & 0 & \ldots & 0 \\
0 & 0 & \chi_u & 0 & \ldots & 0 \\
0 & 0 & 0 & \chi_u & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \ldots & \chi_u \\
\end{pmatrix}
\times E^T,
\]

(18)

at the saddle point. Here, \(E = (e_0, e_1, \ldots, e_n)\) denotes an \(n + 1\)-dimensional orthonormal basis composed of \(e_0 = (1, 0, 0, \ldots, 0)^T\), \(e_1 = (0, n^{-1/2}, n^{-1/2}, \ldots, n^{-1/2})^T\) and \(n - 1\) orthonormal vectors \(e_2, e_3, \ldots, e_n\), which are orthogonal to both \(e_0\) and \(e_1\). Rather laborious but straightforward calculation on the basis of expressions (17) and (18) yields

\[
\lim_{n \to 0} \frac{1}{n} \ln \left[ \exp \left\{ \sum_{a=0}^{n} (w^a)^T X w^a \right\} \right] = A_0(\chi_u, q_u, q_u, m_u, m_u) = F(\chi_u, q_u) + q_u \frac{\partial F}{\partial q_u} + T_w \left( \frac{m_u}{\chi_u} \right)^2 \left( \frac{\langle \lambda \rangle}{2} \right) \frac{\partial F}{\partial \chi_u} - 2m_u \frac{\partial F}{\partial \chi_u},
\]

(19)

where \(T_w = \text{Tr}_w w^2 Q(w)\). This equation and evaluation of the volumes of dynamical variables \(\{w^a\}\) and \(\{w^g\}\) under constraints (15) and (16) of the replica symmetric (RS) ansatz (17) and (18) provide an expression for the average free energy

\[
\frac{1}{N} [\ln Z_F(\Theta_p)]_{\Theta_p} = \frac{1}{n} \ln \left[ Z_F(\Theta_p) \right]_{\Theta_p} = \text{Extr} \left\{ A_0(\chi_u, q_u, q_u, m_u, m_u) + \mathcal{A}_w(\chi_u, q_u, m_u) + \alpha \mathcal{A}_u(\chi_u, q_u, m_u) \right\},
\]

(20)

where \(\Theta = (\chi_u, q_u, q_u, m_u, m_u)\),

\[
\mathcal{A}_w(\chi_u, q_u, m_u) = \text{Extr}_{\chi_u, q_u, m_u} \left\{ \frac{\hat{\chi}_w}{2} (\chi_u + q_u) - \frac{\hat{q}_w}{2} \chi_u - \hat{m}_u m_u \\
+ \text{Tr}_{w^0} Q(w^0) \int Dz \ln \left[ \text{Tr}_w P(w) \exp \left\{ -\frac{\hat{\chi}_w w^2}{2} + (\sqrt{\hat{q}_w z} + \hat{m}_u w^0) w \right\} \right] \right\},
\]

(21)

and

\[
\mathcal{A}_u(\chi_u, q_u, m_u) = \text{Extr}_{\chi_u, q_u, m_u} \left\{ \frac{\hat{\chi}_u}{2} (\chi_u - q_u) + \frac{\hat{q}_u}{2} \chi_u - \hat{m}_u m_u \\
+ \text{Tr}_{y} \int Dz Dz' Q(y) \sqrt{\hat{T}_u - \frac{\hat{m}_u^2}{q_u} x + \frac{\hat{m}_u}{\sqrt{q_u}} z} \ln \left[ \int Dz P(y) \sqrt{\hat{T}_u - \frac{\hat{m}_u^2}{q_u} x + \frac{\hat{m}_u}{\sqrt{q_u}} z} \right] \right\}.
\]

(22)

Here, \(\hat{T}_u = \alpha^{-1} T_u \langle \lambda \rangle\) and \(Dz = ds \exp \left\{ -s^2/2 \right\} \sqrt{2\pi}\) represents the Gaussian measure. Expressions (19)–(22) are the main results of this article.
Two points are noteworthy here. The first is that a set of parameters \( \Theta \) determined by the extremizing equation (20) represents typical macroscopic averages of the posterior distribution (1), by which various performance measures can be evaluated [2]. Moreover, equation (20) itself is linked to information theoretic measures for assessing inference performance. For example, the Kullback-Leibler divergence (per output) between the generative and recognition models, which represents a certain distance from the generative model and is related to the prediction ability of the recognition model for novel data, is evaluated as

\[
KL(Q|P) = \frac{1}{p} \text{Tr} Q(y|X) \ln \frac{Q(y|X)}{P(y|X)} = \frac{1}{\alpha N} [\ln Z_Q(\xi^p)]_{\xi^p} - \frac{1}{\alpha N} [\ln Z_P(\xi^p)]_{\xi^p},
\]

utilizing equation (20) [32]. Equation (20), in conjunction with equation (13), can also be used for calculating the typical mutual information (per output) between the parameter \( w \) and the output \( y \), which represents the information content of \( w \) that can be gained by observing the output \( y \) for typical pattern matrices \( X \), as

\[
I(W; Y) = \frac{1}{p} \frac{1}{w} \text{Tr} Q(w) \prod_{\mu=1}^{p} Q(y_{\mu}|\Delta_{\mu}) \ln \prod_{\mu=1}^{p} Q(y_{\mu}|\Delta_{\mu}) - \frac{1}{p} \frac{1}{y} \text{Tr} Q(y|X) \ln Q(y|X)
\]

\[
= \text{Tr} \int Dz Q(y|\sqrt{T_u} z) \ln Q(y|\sqrt{T_u} z) - \frac{1}{\alpha N} [\ln Z_Q(\xi^p)]_{\xi^p},
\]

specific expressions of which, for problems of communication through additive channels, have been derived in earlier studies [6, 7, 8, 33]. The other issue is that the current formalism can subject to infinitesimal perturbation of the form of the one step RSB yields

\[
\left(1 - 2 \frac{\partial^2 F}{\partial \chi_w^2} \chi_w^{(2)} \right) \left(1 - 2 \frac{\partial^2 F}{\partial \chi_u^2} \chi_u^{(2)} \right) - 4 \frac{1}{\alpha} \left( \frac{\partial^2 F}{\partial \chi_w \partial \chi_u} \right)^2 \chi_w^{(2)} \chi_u^{(2)} < 0,
\]

where

\[
\chi_w^{(2)} = \text{Tr} Q(w^0) \int Dz \left( \frac{\partial^2}{\partial \left( \sqrt{Q_w z} \right)^2} \ln \left[ \text{Tr} P(w) \exp \left[ -\chi_w w^2 + \left( \sqrt{q_w z} + \hat{m}_w w^0 \right) w \right] \right] \right)^2
\]

and

\[
\chi_u^{(2)} = \int Dz Dx Q \left( y|\sqrt{T_u} - \frac{\hat{m}_u}{\sqrt{q_u}} x + \frac{\hat{m}_u}{\sqrt{q_u}} z \right) \times \left( \frac{\partial^2}{\partial \left( \sqrt{Q_u z} \right)^2} \ln \left[ \int Dx P \left( y|\sqrt{\chi_u x} + \sqrt{q_u z} \right) \right] \right)^2.
\]

Equation (25) corresponds to the de Almeida-Thouless (AT) condition for the current system [35].
3.3. The Thouless-Anderson-Palmer approach

The scheme developed so far can be used for macroscopically characterizing the inference performance of equation (1) for typical samples of $\xi^p$. However, another method is necessary to evaluate microscopic averages for an individual sample of $\xi^p$. The Thouless-Anderson-Palmer (TAP) approach [27] known in spin glass research offers a useful guideline for this purpose. Although several formalisms are known for this approximation scheme [4], we here follow the one based on the Gibbs free energy because of its generality and wide applicability [25, 30].

Let us suppose a situation for which the microscopic averages of the dynamical variables

$$m_w = \frac{1}{Z_p(\xi^p)} \text{Tr}_u w P(w|\xi^p) \text{Tr}_u w \prod_{\mu=1}^p \hat{P}_{\mu}(u_{\mu}) \prod_{i=1}^N P(w_i) \exp \left[ iu^T X w \right] ,$$

(28)

and

$$m_u = \frac{1}{Z_p(\xi^p)} \text{Tr}_u u P(u|\xi^p) \text{Tr}_u u \prod_{\mu=1}^p \hat{P}_{\mu}(u_{\mu}) \prod_{i=1}^N P(w_i) \exp \left[ iu^T X w \right] ,$$

(29)

are required. The Gibbs free energy

$$\Phi(m_w, m_u) = \text{Extr}_{h_w, h_u} \{ h_w \cdot m_w + h_u \cdot m_u - \ln [Z_p(h_w, h_u)] \} ,$$

(30)

where

$$Z_p(h_w, h_u) = \text{Tr}_u \prod_{\mu=1}^p \hat{P}_{\mu}(u_{\mu}) \prod_{i=1}^N P(w_i) \exp \left[ h_w \cdot w + h_u \cdot (iu) + (iu)^T X w \right] ,$$

(31)

offers a useful basis for this objective as the extremization conditions of equation (30) generally agree with equations (28) and (29). This indicates that one can evaluate the microscopic averages (28) and (29) by extremization once the function of Gibbs free energy (30) is provided.

Unfortunately, exact evaluation of equation (30) is computationally difficult and therefore we resort to approximation. For this purpose, we put a parameter $l$ in front of $X$ in equation (31), which yields the generalized Gibbs free energy as

$$\bar{\Phi}(m_w, m_u; l) = \text{Extr}_{h_w, h_u} \{ h_w \cdot m_w + h_u \cdot m_u - \ln [Z_p(h_w, h_u; l)] \} ,$$

(32)

where $Z_p(h_w, h_u; l) = \text{Tr}_u \prod_{\mu=1}^p \hat{P}_{\mu}(u_{\mu}) \prod_{i=1}^N P(w_i) \exp \left[ h_w \cdot w + h_u \cdot (iu) + (iu)^T (lX) w \right]$. This implies that the correct free energy (30) can be obtained as $\Phi(m_w, m_u) = \bar{\Phi}(m_w, m_u; l = 1)$ by setting $l = 1$ in the generalized expression (32). One scheme to make use of this relation is to perform the Taylor expansion around $l = 0$, for which $\bar{\Phi}(m_w, m_u; l)$ can be analytically calculated as an exceptional case, and substitute $l = 1$ in the expression obtained, which is sometimes referred to as the Plefka expansion [36]. However, evaluation of higher order terms, which are not negligible for correlated patterns in general, requires a complicated calculation in this expansion, which sometimes prevents the scheme from being practically tractable. In order to avoid this difficulty, we take an alternative approach here, which is inspired by a derivative of equation (32)

$$\frac{\partial \bar{\Phi}(m_w, m_u; l)}{\partial l} = - \langle (iu)^T X w \rangle_l ,$$

(33)
Extremization of this equation provides a set of TAP equations where constrained as of equation (33) using a Gaussian distribution for which the first and second moments are to satisfy \( \langle \mathbf{w} \rangle_l = \mathbf{m}_w \) and \( \langle \mathbf{i} \mathbf{u} \rangle_l = \mathbf{m}_u \), respectively [25]. The right hand side of this equation is an average of a quadratic form containing many random variables. The central limit theorem implies that such an average does not depend on details of the objective distribution but is determined only by the values of the first and second moments. In order to construct a simple approximation scheme, let us assume that the second moments are characterized macroscopically by \( \langle |\mathbf{w}|^2 \rangle_l - \langle |\mathbf{w}|^2 \rangle_l = N \chi_w \) and \( \langle |\mathbf{u}|^2 \rangle_l - \langle |\mathbf{u}|^2 \rangle_l = p \chi_u \). Evaluating the right hand side of equation (33) using a Gaussian distribution for which the first and second moments are constrained as \( \langle \mathbf{w} \rangle_l = \mathbf{m}_w \), \( \langle \mathbf{i} \mathbf{u} \rangle_l = \mathbf{m}_u \), \( \langle |\mathbf{w}|^2 \rangle_l - \langle |\mathbf{w}|^2 \rangle_l = N \chi_w \) and \( \langle |\mathbf{u}|^2 \rangle_l - \langle |\mathbf{u}|^2 \rangle_l = p \chi_u \), and integrating from \( l = 0 \) to \( l = 1 \) yield

\[
\tilde{\Phi}(\chi_w, \chi_u, \mathbf{m}_w, \mathbf{m}_u; 1) - \tilde{\Phi}(\chi_w, \chi_u, \mathbf{m}_w, \mathbf{m}_u; 0) \simeq -m_u^T X m_w - NF(\chi_w, \chi_u),
\]

where the function \( F(x, y) \) is provided as in equation (9) by the empirical eigenvalue spectrum of \( X^T X \), \( \rho(\lambda) = N^{-1} \sum_{k=1}^{N} \delta(\lambda - \lambda_k) \) and the macroscopic second moments \( \chi_w \) and \( \chi_u \) are included in arguments of the Gibbs free energy as the right hand side of equation (33) depends on them. Utilizing this and evaluating \( \tilde{\Phi}(\chi_w, \chi_u, \mathbf{m}_w, \mathbf{m}_u; 0) \), which is not computationally difficult since interaction terms are not included, offer an approximation of the Gibbs free energy as

\[
\Phi(\chi_w, \chi_u, \mathbf{m}_w, \mathbf{m}_u) \simeq -m_u^T X m_w - NF(\chi_w, \chi_u)
\]

\[
+ \text{Extr}_{\tilde{\chi}_w, \mathbf{h}_w} \left\{ h_w \cdot m_w - \frac{1}{2} \tilde{\chi}_w \left( N \chi_w + |\mathbf{m}_w|^2 \right) - \sum_{i=1}^{N} \ln \left[ \text{Tr} P(w) e^{-\frac{1}{2} \tilde{\chi}_w w^2 + h_w w} \right] \right\}
\]

\[
+ \text{Extr}_{\tilde{\chi}_u, \mathbf{h}_u} \left\{ h_u \cdot m_u - \frac{1}{2} \tilde{\chi}_u \left( p \chi_u - |\mathbf{m}_u|^2 \right) - \sum_{\mu=1}^{p} \ln \left[ \int D\mathbf{x} P(y_{\mu} | \sqrt{\chi_u} x + h_{u\mu}) \right] \right\},
\]

which is a general expression of the TAP free energy of the current objective system (1). Extremization of this equation provides a set of TAP equations

\[
m_{wi} = \frac{\partial}{\partial h_{wi}} \ln \left[ \text{Tr} P(w) e^{-\frac{1}{2} \tilde{\chi}_w w^2 + h_w w} \right],
\]

\[
\chi_w = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial^2}{\partial h_{wi}^2} \ln \left[ \text{Tr} P(w) e^{-\frac{1}{2} \tilde{\chi}_w w^2 + h_w w} \right],
\]

\[
m_{u\mu} = \frac{\partial}{\partial h_{u\mu}} \ln \left[ \int D\mathbf{x} P(y_{\mu} | \sqrt{\chi_u} x + h_{u\mu}) \right],
\]

\[
\chi_u = -\frac{1}{p} \sum_{\mu=1}^{p} \frac{\partial^2}{\partial h_{u\mu}^2} \ln \left[ \int D\mathbf{x} P(y_{\mu} | \sqrt{\chi_u} x + h_{u\mu}) \right],
\]

where

\[
h_w = X^T m_u - 2 \frac{\partial}{\partial \chi_w} F(\chi_w, \chi_u) m_w,
\]

\[
\tilde{\chi}_w = -2 \frac{\partial}{\partial \chi_w} F(\chi_w, \chi_u),
\]

\[
h_u = X m_w + 2 \frac{\partial}{\partial \chi_u} F(\chi_w, \chi_u) m_u,
\]

\[
\tilde{\chi}_u = -2 \frac{\partial}{\partial \chi_u} F(\chi_w, \chi_u),
\]
solutions of which represent approximate values of the first and second moments of the distribution (1) for a fixed sample of $X$ (or $\xi^p$). $-2(\partial/\partial \chi_w)F(\chi_w, \chi_u)m_w$ and $(2/\alpha)(\partial/\partial \lambda)F(\chi_w, \chi_u)m_u$ in equations (40) and (42) are generally referred to as the Onsager reaction terms. Counterparts of these equations for systems of two-body interactions have been presented in an earlier article [30]. Although we have assumed single macroscopic constraints as characterizing the second moments, the current formalism can be generalized to include component-wise multiple constraints for constructing more accurate approximations, which leads to the adaptive TAP approach or, more generally, the expectation consistent approximate schemes developed by Opper and Winther [23, 24, 25].

4. Examples
4.1. Patterns of independently and identically distributed entries
In order to investigate the relationship with existing results, let us first employ the developed methodologies to the case in which the entries of $X$ are independently drawn from an identical distribution with zero mean and variance $N^{-1}$. This case is characterized by an eigenvalue spectrum of Marčenko-Pastur type, $\rho(\lambda) = [1 - \alpha^+ \delta(\lambda) + (2\pi)^{-1}\lambda^{-1}\sqrt{[\lambda - \lambda_-]^+ [\lambda_+ - \lambda]^+}$, where $[x]^+ = x$ for $x > 0$ and 0, otherwise, and $\lambda_{\pm} = (\sqrt{\alpha} \pm 1)^2$ [20], which yields

$$F(x, y) = -\frac{\alpha}{2} xy. \quad (44)$$

This together with the relation $\langle \lambda \rangle_\rho = \alpha$, which holds for the current eigenvalue spectrum, implies that equation (19) can be expressed as

$$A_0(\chi_w, \chi_u, q_w, q_u, m_w, m_u) = -\frac{\alpha}{2} (\chi_w \chi_u + q_w \chi_u - q_u \chi_w - 2m_w m_u). \quad (45)$$

Inserting this into equation (20) and then performing an extremization with respect to $\chi_u$, $q_u$ and $m_u$ yields

$$\hat{\chi}_u = \chi_u, \quad \hat{q}_u = q_u, \quad \hat{m}_u = m_u, \quad (46)$$

where $\hat{\chi}_u$, $\hat{q}_u$ and $\hat{m}_u$ are the variational variables used in equation (22). This implies that the replica symmetric free energy (20) can be expressed as

$$\frac{1}{N} [\ln Z_P(\xi^p)]_{\xi^p} = \frac{\text{Extr}}{\chi_w, q_w, m_w} \left\{ A_w(\chi_w, q_w, m_w) + \alpha \text{Tr} \int Dz D\lambda \left( y \left[ T_w - \frac{m_w^2}{q_w} x + \frac{m_w q_w}{\sqrt{q_w}} \right] \ln \left[ \int Dz P(y \sqrt{\chi_w x + \sqrt{q_w z}}) \right] \right) \right\}, \quad (47)$$

where the relation $T_w = \alpha^{-1} \langle \lambda \rangle_\rho T_w$ was utilized. This is equivalent to the general expression of the replica symmetric free energy of a single layer perceptron for pattern matrices with independently and identically distributed entries [2, 37].

4.2. Gaussian linear vector channel
The second example to show equivalent results to those obtained by earlier analysis is that of a Gaussian linear vector channel, which is characterized by $P(y|\Delta) = (2\pi \sigma^2)^{-1/2} \exp \left\{ -(y - \Delta)^2 /(2\sigma^2) \right\}$ and $Q(y|\Delta) = (2\pi \sigma_0^2)^{-1/2} \exp \left\{ -(y - \Delta)^2 /(2\sigma_0^2) \right\}$. In this case, equation (22) is evaluated as

$$A_u(\chi_u, q_u, m_u) = \frac{1}{2} \left( \sigma^2 - \frac{1}{\chi_u} \right) q_u - \frac{1}{2} \left( \sigma^2 \chi_u - \ln \chi_u - 1 \right) - \frac{1}{2} \chi_u (\hat{T}_u + \sigma_0^2), \quad (48)$$
while requiring that \( m_u/\chi_u = 1 \). Further, extremization with respect to \( q_u \) in equation (20) indicates that \( \Lambda_\chi \), which is the counterpart of \( \Lambda_y \) in equation (9) for \( y = \chi_u \), is set to a constant value \( \Lambda_\chi = \sigma^2 \), which implies that \( (\partial/\partial \chi_u) F(\chi_w, \chi_u) = (1/2)(\sigma^2 - \chi_u^{-1}) \) and \( \chi_u = \sigma^{-2} + 2(\alpha \sigma^2)^{-1} \chi_u (\partial/\partial \chi_u) F(\chi_w, \chi_u) \) hold. These, in conjunction with \( \alpha T_u = T_w \langle \lambda \rangle_p \), indicate that equation (20) can be expressed as

\[
\frac{1}{N} \left[ \ln Z_P(\xi^p) \right]_{p} = \operatorname{Extr}_{\chi_w, q_w, m_w} \left\{ A_w(\chi_w, q_w, m_w) \right\} + G \left( \frac{\chi_w}{\sigma^2} \right) + \left( -\frac{T_w - 2m_w + q_w}{\sigma^2} + \frac{\sigma^2}{\sigma^4} - \frac{1}{2} \right) G' \left( -\frac{\chi_w}{\sigma^2} \right) - \frac{\alpha}{2} \left( \ln(2\pi \sigma^2) + \frac{\sigma^2}{\sigma^4} \right),
\]

where

\[
G(x) = \operatorname{Extr}_{\Lambda} \left\{ -\frac{1}{2} \langle \ln(\Lambda - \lambda) \rangle_p + \frac{\Lambda}{2} x \right\} - \frac{1}{2} \ln x - \frac{1}{2},
\]

is referred to as the Itzykson-Zuber integral or \( G \)-function in physics literature [28, 29, 30, 31], which is linked to the \( R \)-transform of the cross-correlation matrix \( X^T X \) used in free probability theory [20, 38, 39]. Equation (49) is equivalent to the expression for the replica symmetric free energy for Gaussian linear vector channels of a correlated channel matrix recently provided by the author and his colleagues [21, 22].

4.3. Ability of the Ising perceptron to separate random orthogonal patterns

In order to demonstrate the utility of the methodologies we have developed, as our final example we take up a simple but nontrivial problem concerning the separation ability of the Ising perceptron. Let us consider a simple perceptron of binary weight \( w = \{+1, -1\}^N \), \( P(y|\Delta) = 1 \) for \( y\Delta > 0 \) and 0, otherwise, where \( y = \pm 1 \). It is known that, in typical cases, this network can correctly separate a set of random patterns \( \xi^p = \{(x_1, y_1), (x_2, y_2), \ldots, (x_p, y_p)\} = (X, y) \) up to \( \alpha_c \approx 0.833 \), when the elements of \( x_\mu \) are independently generated from an isotropic distribution and the elements of \( y_\mu = \pm 1 \) are independently and randomly assigned with a probability of one half for \( \mu = 1, 2, \ldots, p \) [40, 41, 42]. Our question here is how \( \alpha_c \) is modified when the pattern matrix \( X \) is generated randomly in such a way that the patterns \( x_\mu \) are orthogonal to each other. In order to answer this question, we employ the replica and TAP methods developed in preceding sections for \( \rho(\lambda) = (1 - \alpha)\delta(\lambda) + \alpha \delta(\lambda - 1) \), which represents the eigenvalue spectrum of the random orthogonal patterns, assuming \( 0 < \alpha < 1 \). Figure 1 shows how the entropy of \( w \) depends on the pattern ratio \( \alpha \). The curve indicates the theoretical prediction of the replica analysis while the markers denote the averages of entropy obtained by the TAP method over 100 samples for \( N = 500 \) systems. The error bars are smaller than the markers. Solutions of the TAP method are obtained by an algorithm of message-passing type, details of which are reported elsewhere [43]. Although the curve and the markers exhibit excellent agreement for the data points \( \alpha = 0.1, 0.2, \ldots, 0.8 \), we were not able to obtain a reliable result for \( \alpha = 0.9 \), at which the message-passing algorithm does not converge in most cases even after 1000 iterations. This may be a consequence of RSB since the replica analysis indicates that the AT stability is broken at \( \alpha_{\text{AT}} \approx 0.810 \). Therefore \( \alpha_c \approx 0.940 \) indicated by the condition of vanishing entropy is to be regarded not as the exact but as an approximate value provided by the unstable RS solution. However, extrapolation from the results of direct numerical experiments for finite size systems indicates that \( \alpha_c \approx 0.938 \) [43], which implies that the effect of RSB is not significant for the evaluation of \( \alpha_c \) in this particular case.

5. Summary

We have developed a framework for analyzing the inference performance of densely-connected single-layer networks, typical examples of which are perceptrons and models of linear vector
channels. The development is intended for dealing with correlated patterns. For this purpose, we have developed two methodologies based on the replica method and the Thouless-Anderson-Palmer approach, which are standard tools from the statistical mechanics of disordered systems, introducing a certain random assumption about the singular value decomposition of the pattern matrix. The validity and utility of the developed schemes are shown for two existing results and a novel problem.

Investigation of the properties of algorithms for solving the TAP equations (36)–(43) [14, 17, 18] and variants of them [15, 16, 44], as well as application of the developed framework to real world data analysis [45, 46] and various channel models [19, 20], are promising topics for future research.

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