Estimation for High-Dimensional Multi-Layer Generalized Linear Model – Part I: The Exact MMSE Estimator

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Abstract—This two-part work considers the minimum means square error (MMSE) estimation problem for a high dimensional multi-layer generalized linear model (ML-GLM), which resembles a feed-forward fully connected deep learning network in that each of its layers mix up the random input with a known weighting matrix and activates the results via non-linear functions, except that the activation here is stochastic and following some random distribution. Part I of the work focuses on the exact MMSE estimator, whose implementation is long known infeasible. For this exact estimator, an asymptotic analysis on the performance is carried out using a new replica method that is refined from certain aspects. A decoupling principle is then established, suggesting that, in terms of joint input-and-estimate distribution, the original estimation problem of multiple-input multiple-output is indeed identical to a simple single-input single-output one subjected to additive white Gaussian noise (AWGN) only. The variance of the AWGN is further shown to be determined by some coupled equations, whose dependency on the weighting and activation is given explicitly and analytically. Comparing to existing results, this paper is the first to offer a decoupling principle for the ML-GLM estimation problem. To further address the implementation issue of an exact solution, Part II proposes an approximate estimator, ML-GAMP, whose per-iteration complexity is as low as GAMP, while its asymptotic MSE (if converged) is as optimal as the exact MMSE estimator.

Index Terms—multi-layer GLM (ML-GLM), minimal mean square error (MMSE), replica method, generalized approximated message passing (GAMP), multiple-input multiple-output (MIMO)

I. INTRODUCTION

This paper considers the problem of estimating high dimensional random inputs from their observations obtained from a multi-layer generalized linear model (ML-GLM) [1]:

\[ y = f_L(H_L \cdots f_2(H_2f_1(H_1x; \eta_1)\cdots; \eta_2)\cdots; \eta_L) \]

in which \( x \) the is high dimensional random input, \( y \) is the high dimensional observation, \( H_\ell \) is the weighting matrix in the \( \ell \)-th layer (\( \ell = 1, \ldots, L \)) that linearly combines its input, and \( f_\ell(x; \eta_\ell) = \prod_{a=1}^{M} f_\ell(x_a; \eta_{\ell,a}) \) is the activation function that maps the weighted result componentwisely. The model, ML-GLM, resembles a feed-forward deep learning network of full connections in many aspects, except that the activation here is random. In particular, the activation here has a parameter \( \eta_\ell \) that follows some random distribution, and as a consequence, the entire activation process requires a transitional distribution to fully characterize its input-output relation. To see how this differs from a classical neural network, consider a case where the (deterministic) bias is replaced by some random values drawn from a Gaussian population. The activated result in that case is no longer deterministic due to the random bias, even though the activation in itself is deterministic. The ML-GLM is a general model, embracing many well-known models as special cases. For instance, when \( L = 1 \), it reduces to the generalized linear model (GLM) [2], [3], a model described by \( y = f(Hx; \eta) \) and extensively adopted in low-resolution quantization studies [4] where \( y = \text{ADC}(Hx + \eta) \) with \( \text{ADC}(\cdot) \) modeling the analog-to-digital conversion. As another instance, when the random activation is modeled by some additive white Gaussian noise (AWGN), the ML-GLM reduces to the celebrated standard linear model (SLM) [5], where \( y = Hx + \eta \) and its applications have a wide range of varieties, including wireless communications [6], image processing [7], compressive sampling [5], and many others. As a generalization to the above models, the general ML-GLM is further able to model the inference problem arising in deep learning applications [8].

For these models, the estimation problem is a classic yet still active topic, to which tremendous efforts had been dedicated during the past few decades. Among these is the minimum mean square error (MMSE) estimator, which is optimal in the MSE sense as its output \( \hat{x} \) could minimize \( \mathbb{E}[\|x - \hat{x}\|^2] \). The exact implementation of an MMSE estimator, however, is infeasible [9] (NP-hard) in high dimensional latent space, because of its requirements on the marginalization of a posterior distribution that contains many random variables or on the expectations over these distributions. This issue was recognized as a facet of the curse of dimensionality, and as a remedy, people started to look at approximate solutions. Among those scaling well to high-dimensional applications, approximate message passing (AMP) [5] enjoyed a great popularity in scenarios with known and factorable priors. Originally designed for compressive recovery in the SLM setting, AMP was able to offer a Bayes-optimal estimation performance (it achieved the theoretical bound of a sparsity-undersampling tradeoff) but its implementation complexity is
kept at a surprisingly low level (its message number scaled linearly with the variable number per iteration). Following AMP, a great number of approximate solutions had been proposed, and among these were three estimators pertaining to ML-GLM and thus are of particular interest here. The three are generalized AMP (GAMP) \[2\], multi-layer AMP (ML-AMP) \[1\], and multi-layer vector AMP (ML-VAMP) \[8\]. The first estimator, GAMP \[2\], extended AMP’s scope (SLM) to allow non-linear activation (GLM); however, it considered only a single layer. As more recent advances, the latter two, ML-AMP \[1\] and the ML-VAMP \[8\], were able to handle the multi-layer case, but they also suffered from some limitations. In particular, the ML-VAMP \[8\] required a singular value decomposition (SVD) on each of the weighting matrices and thus inevitably comprised its computational efficiency, while the ML-AMP \[1\], although more efficient in computation (as no SVD needed), converged in a relatively slow speed (as one will see from our simulation section in Part II).

To fill in this gap, this two-part work proposes a new estimator, the ML-GAMP, whose convergence rate turns out to be faster than ML-AMP \[1\] (by using messages that are not SVD needed), converged in a relatively fast speed (as one will see from our simulation section in Part II).

Below, we summarize two major findings of this Part I paper: to the (lengthy) replica analysis of an exact MMSE estimator, the ML-AMP \[1\], although more efficient in computation (as no SVD needed), converged in a relatively slow speed (as one will see from our simulation section in Part II).

II. SYSTEM MODEL AND PROBLEM FORMULATION

Fig.1 is an illustration for the MMSE estimation in an ML-GLM setting. In the figure, \(x_0\) denotes the initial random input, whose distribution is factorable and known by the estimator, i.e., \(x_0 \sim \mathcal{P}_X(x_0) = \prod_{i=1}^{N_1} \mathcal{P}_X(x_0_i)\). \(y\) denotes the observation attained from the ML-GLM network of \(L\) layers, and \(\{x\}\) is the output generated by the MMSE estimator, in an manner either exact or approximate. Particularly, the \(\ell\)-th layer expands as (1 \(\leq \ell \leq L\)

\[
\rightarrow x^{(\ell)} \rightarrow H^{(\ell)}x^{(\ell)} \rightarrow z^{(\ell)} \rightarrow \mathcal{P}(x^{(\ell+1)}|z^{(\ell)}) \rightarrow x^{(\ell+1)} \rightarrow (2)
\]

where \(x^{(\ell)} \in \mathbb{R}^{N_\ell}\) is its input, and \(H^{(\ell)} \in \mathbb{R}^{N_{\ell+1} \times N_{\ell}}\) is a deterministic weighting matrix that linearly mixes up the input to yield \(z \in \mathbb{R}^{N_{\ell+1}}\). This weighted result \(z\) is then activated by a random mapping, whose transition/conditional probability density function (p.d.f.) is also factorable: \(\mathcal{P}(x^{(\ell+1)}|z^{(\ell)}) = \prod_{a=1}^{N_{\ell+1}} \mathcal{P}(x_{a}^{(\ell+1)}|z_{a}^{(\ell)})\). The weighting matrix above is known perfectly to the estimator, and in each experiment, the elements of this matrix are drawn independently from the same Gaussian ensemble of zero mean and \(1/N_{\ell+1}\) variance (to ensure a unit row norm). To maintain notational consistency, we also initialize: \(x^{(1)} := x_0\), and \(x^{(L+1)} := y\). Since we consider exclusively the limiting performance of the MMSE estimators, the following assumptions are made throughout the paper: \(N_{\ell} \rightarrow \infty\) while \(N_{\ell+1}/N_{\ell} \to \alpha_{\ell}\), i.e., all weighting matrices are sufficiently large in size, but the ratios of their row numbers to column numbers are fixed and bounded\[1\].

The target of an exact MMSE estimator is to generate an estimate \(\{\hat{x}_k\}\) for every input element \(x_{0k}\) using \((k = 1, \cdots, N_1)\)

\[
\{\hat{x}_k\} = \arg\min_{\hat{x}_k} \mathbb{E} \left[ \|\hat{x}_k - x_k\|^2 \right] = \mathbb{E} \left[ x_k | y, \{H^{(\ell)}\} \right] \quad (3)
\]

where the last expectation is taken over a marginal posterior

\[
\mathcal{P}(x_{0k}|y, \{H^{(\ell)}\}) = \int \mathcal{P}(x_{0}|y, \{H^{(\ell)}\})|dx_{0},\quad (4)
\]

whose integration is \((N_{1} - 1)\)-fold, \(x_{0k}\) equals \(x_0\) except its \(k\)-th element moved, and the joint p.d.f. \(\mathcal{P}(x_{0}|y, \{H^{(\ell)}\})\) is:

\[
\mathcal{P}(x_{0}|y, \{H^{(\ell)}\}) = \int \mathcal{P}_X(x_0)\mathcal{P}(y|x_0, \{H^{(\ell)}\})|dx_{0} = \int \mathcal{P}_X(x_0)\mathcal{P}(y|x_0, \{H^{(\ell)}\})|dx_{0}.
\]

For the above MMSE estimator, we note that its exact implementation requires the evaluation of a multi-fold integral as above. In high dimensional scenarios, this is apparently
infeasible. For performance analysis, we also note that, this
two-part work adopts the average MSE defined as:
\[
\text{avgMSE} \triangleq \frac{1}{N_0} \sum_{k=1}^{N_1} E \left[ \| x_k - \hat{x}_k \|^2 \right],
\]
i.e., an average of MSE realizations over all input \( x \), weighting \( \{H^{(k)}\} \), and activation \( \{P(x^{(k)}|\hat{z}^{(k)})\} \) randomness.

Next, we start from a relatively simple case of 2L-GLM to
analyze the exact MMSE estimator’s performance. Its result
will be extended to more general cases in subsequent sections.

III. ASYMPTOTIC ANALYSIS FOR TWO-LAYER CASE

To ease statement, we adopt a new set of notations in this
two-layer section, hoping it to save us from the ocean of
superscripts. To be specific, we re-define 2L-GLM as below:
\[
x_0 \rightarrow Hx_0 \rightarrow u \rightarrow P(s|u) \rightarrow s \rightarrow C_s \rightarrow v \rightarrow y
\]
with \( P(s|u) \) and \( P(y|v) \) denoting the new random activation
in the two layers. The MMSE estimate of \( x_0 \)'s \( k \)-th element
then becomes:
\[
\langle x_k \rangle = E \left[ x_0|k, y, C, H \right],
\]
where the expectation is taken over \( P(x_0|y, H, C) \), i.e., the marginal of a joint posterior given by
\[
P(x_0|y, C, H) = \frac{P_X(X_0)P(y|x_0, C, H)}{P_Y(Y|x)}.
\]
Under this new 2L-GLM notations, the system model is illustrated as Fig. 2(a). Next, we present
the main result from our replica analysis, while leaving its
derivation details to the remainings subsections.

A. Results for Exact MMSE Estimator in 2L-GLM

Claim 1 (Joint distribution: 2-layer). As illustrated in Fig. 2,
\[
(x_{0k}, \langle x_k \rangle) \cong (X_0, \langle X \rangle), \quad \forall k,
\]
which means the exact MMSE estimation in a MIMO 2L-GLM:
\[
x_0 \xrightarrow{P(y|x_0, C, H)} y \xrightarrow{E_{x_0|y}(x_0)} \langle x \rangle
\]
is identical, in terms of joint input-and-estimate distribution,
to that in a SISO setting with only an (effective) AWGN:
\[
X_0 \xrightarrow{W} Y \xrightarrow{E_X(X)} \langle X \rangle
\]
where \( X_0 \sim P_X(X_0) \) is a scalar input following the same
distribution as an element \( x_{0k} \) of the original vector \( x_0 \),
\( Y = X_0 + W \) is the scalar received signal only corrupted
by an AWGN, \( W \sim N(0, \sigma^2) \), and \( \langle X \rangle \) is the scalar MMSE
estimate obtained via \( \langle X \rangle \triangleq \mathbb{E}_{X_0}|Y[X_0] \) with
\( P(X_0|Y) = \frac{P_X(X_0)N(Y|X_0, \sigma^2)}{P_Y(Y|x_0, a)}x_0 \). The noise variance \( \eta \) could be further
determined from the solution to the coupled equations \([12]\)
below, using the relation \( \eta \equiv 1/(2\hat{d}) \). Let \( \sigma_w^2 \) denote
the variance of \( P_X(x, a) \), \( N(x|a, A) \) be a Gaussian density of mean \( a \)
and covariance (matrix) \( A \), \( \mathbb{D}_x \triangleq \mathbb{N}(x, 0, 1)d^2 \) be a Gaussian
measure, and \( N_{\hat{d}}(a, b, B) \triangleq \mathbb{P}(s|u)N(s|a, A)N(u|b, B) \),
the coupled equations then read
\[
c = \sigma_X^2
\]
\[
e = \int_{a} \int_{d} |s|^2 P(s|u)N(0, \frac{1}{\alpha}) du ds
\]
\[
h = \int_{a} \int_{d} \int_{v} \int_{f} \mathbb{P}(y|v)N(0, \frac{1}{\alpha}) du dv df dv
\]
\[
\hat{f} = \frac{\beta(h - f)}{2(e - f)^2}
\]
\[
q = \int_{a} \int_{d} \int_{v} \int_{f} \mathbb{P}(y|v)N(0, \frac{1}{\alpha}) du dv df dv
\]
\[
d = \alpha(\alpha q - d) \frac{1}{2(e - f)^2}
\]
\[
f = \int_{a} \int_{d} \int_{v} \int_{f} \mathbb{P}(y|v)N(0, \frac{1}{\alpha}) du dv df dv
\]
for the more general ML-GLM case, an in-depth analysis is omitted here due to limited space and left to further studies.

**Remark 2:** The above claim was obtained from a replica analysis (with certain refinements), whose details will be given in subsequent subsections. Inside the wireless communication community, related pioneering work include [15] by Tanaka, [12] by Guo and Verdú, and their collaboration [16], but considering a CDMA application. In a more recent line of works, the replica method was to apply to the analysis of compressive sensing [17] by Kabashima et al., MIMO [18] by Wen et al., and massive MIMO [19] by Wen et al. All these work, however, concentrated on a single-layer setup, and the more general (also more challenging) ML-GLM was not considered until a recent work [1] by Manoel et al. Comparing to [12] and [1], Claim [1] on one hand, substantially extends the decoupling principle established by [12] in a single-layer linear setting (SLM) to the much more general setting (ML-GLM) of multiple layers and non-linearity. On the other hand, it provided more details about the inner structure of the fixed point equations, as compared to [1]. The above extension from 1L-SLM to ML-GLM is no trivial work, because (as discussed later) a key step in [12] is to compute certain point equations, as compared to [1].

**Remark 3:** The coupled equations in Claim [1] may have multiple solutions, which was recognized as phase coexistence in the literature. In statistical physics, as the system’s parameters change, the dominant solution of the system may switch from one coexisting solution to another (thus termed phase transition), and the thermodynamically dominant solution is the one that gives a smallest free energy value [16]. While in the wireless communications context, a solution carrying the most relevant operational meaning is the one that yields an optimal spectral efficiency [12].

**Remark 4:** From the discussion around (85), two quantities from Claim [1], and, have some interesting interpretation: $c = \mathbb{E}[X^2]$ equals the power of a single input element, and $d = \mathbb{E}[(X)^2]$ equals the power of its corresponding estimate. A natural idea from this interpretation is that, to evaluate the average MSE of a system, one only needs to compute a simple subtraction $c - d$, i.e.,

$$\text{avgMSE} = c - d. \quad (14)$$

meaning that given $c$ and $d$, one could be saved from the trouble of time-consuming Monte Carlo simulations that mimic the entire process of data generation, ML-GLM processing, MMSE estimation, and even error counting. To prove (14), we start from the average MSE’s definition: $\text{avgMSE} \triangleq \mathbb{E}[(X - \langle X \rangle)^2]$ ($\langle \rangle$ applies the orthogonality principle from MMSE estimators, which says that, $\langle (X - \langle X \rangle) \rangle$, the error vector of the MSE-optimal estimator is orthogonal to any possible estimator, including $\langle X \rangle$ itself. Given $c$ and $d$, eq. (14) could give the average MSE without simulations; this is one side of the coin. On the other side, in case of $d$ not available, eq. (14) could give $d = c - \text{avgMSE}(d)$, saving us from the two-fold integral of (15), where the dependency of the average MSE on a known quantity $d$, defined in (15), is explicitly given by $\text{avgMSE}(d)$. An analytical expression for the dependency is possible, e.g., if the prior $\mathcal{P}_X(x)$ takes a QPSK form, then the average MSE could be rewritten explicitly as [20]: $\text{avgMSE}(d) = 1 - f \tanh(2d + \sqrt{2}dz)dz$, recalling $\eta = 1/(2d)$. Given the average MSE, it is also possible to compute numerically other performance indices. Take the symbol error rate (SER) as an example, if the transmitted symbol $X$ is drawn from a QPSK constellation, then the conversion from MSE to SER could be expressed analytically as [21] p. 269 SER = $2Q(\sqrt{\eta}) - [Q(\sqrt{\eta})]^2$, where

\[ f(0, P^*, Q^*) = 0, \frac{\partial}{\partial P^*} f(0, P^*, Q^*) = 0, \quad (13) \]

\[ \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \max_{P} \min_{Q} f(\tau, P, Q) = \lim_{\tau \to 0} \max_{P} \min_{Q} \frac{\partial}{\partial \tau} f(\tau, P, Q). \]

However, such an interchange had seldom been justified, and counter examples around in the mathematical world, if the function $f$ is arbitrary. Noticing this, we follow a different procedure to handle the evaluation, which retains the analytical tractability but at the same time is also rigorous mathematically. It reads here

\[ \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \max_{P} \min_{Q} f(\tau, P, Q) = \lim_{\tau \to 0} \frac{\partial}{\partial \tau} f(\tau, P^*, Q^*) \quad (12) \]

with $(P^*, Q^*)$ being a solution to the following equation set

\[ \frac{\partial}{\partial P^*} f(0, P^*, Q^*) = 0, \quad \frac{\partial}{\partial Q^*} f(0, P^*, Q^*) = 0. \quad (13) \]

\[ \text{avgMSE} = c - d. \quad (14) \]

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where the last equality follows from a self-averaging property of the high-dimensional signals \([12, 23]\). Next, we show that

\[
\text{r.h.s.} \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \log \mathbb{E}_{x_0, y, C, H}[\mathcal{L}^{(\tau)}(y, C, H, x_0; h)] \quad (22)
\]

\[
\mathcal{L}^{(\tau)}(\cdot) = \mathbb{E}_{x_0}[\cdot]
\]

\[
\exp\left(\frac{h}{K} \sum_{k=1}^{K} x_{0k} \prod_{u=1}^{j} x_{uk} \cdot \prod_{a=1}^{\tau} \mathcal{P}(y|x_a, C, H)\right)
\]

where \(\{x_a\} \triangleq \{x_1, \ldots, x_{\tau}\}\). The proof for (22) starts from an expansion on its r.h.s.. Substituting \(\mathcal{L}^{(\tau)}(\cdot)\) back into the formula and evaluate the partial derivative at its limit yields

\[
\text{r.h.s.} \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \log \mathbb{E}_{x_0, y, C, H}[\mathcal{L}^{(\tau)}(y, C, H, x_0; h)] = \text{r.h.s.} \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \log \mathbb{E}_{x_0, y, C, H}[\mathcal{L}^{(\tau)}(y, C, H, x_0; h)]
\]

which completes the proof for (22). So far, we have proved

\[
\text{l.h.s.} \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \log \mathbb{E}_{x_0, y, C, H}[\mathcal{L}^{(\tau)}(y, C, H, x_0; h)] = \text{l.h.s.} \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \log \mathbb{E}_{x_0, y, C, H}[\mathcal{L}^{(\tau)}(y, C, H, x_0; h)]
\]

Then, based on (24), we continue to evaluate

\[
\frac{1}{K} \log \mathbb{E}_{x_0, y, C, H}[\mathcal{L}^{(\tau)}(y, C, H, x_0; h)]
\]

\[
= \text{Extr}_{Q_S, Q_X} G^{(\tau)}(Q_S) - \alpha \text{tr}(Q_S Q_X) + \beta \mathcal{O}(Q_X) - R^{(\tau)}(Q_X; h) \quad (25)
\]

where the proof for the result of (25) will be given immediately in next subsection (Step 1 and 2). ‘Extr’ denotes an extreme value operation. \(Q_X, Q_X, Q_S\) and \(Q_S, Q_X\) are all \((\tau+1) \times (\tau+1)\) matrices. \(G^{(\tau)}(Q_S)\) and \(G^{(\tau)}(Q_S, Q_X)\) are defined around (24). \(R^{(\tau)}(Q_X; h)\) is the rate function of a density below:

\[
\mathcal{P}(Q_X; h) \triangleq \mathbb{E}_{x_0, \{x_a\}}\left(\frac{h}{K} \sum_{k=1}^{K} x_{0k} \prod_{u=1}^{j} x_{uk} \cdot \prod_{a=1}^{\tau} \delta_{a,b}\right) \quad (27)
\]
where $\delta_{a,b} \triangleq \delta \left( \sum_{k=1}^{K} x_{ak} x_{bk} - K Q_{X} a b \right)$ with $Q_{X} a b$ being the $(a, b)$-th element of $Q_{X}$. This rate function could be given explicitly using the large deviation theory as \cite{12} B-VI:

$$R(\tau) (Q_{X}; h) = \sup \left\{ \nu(Q_{X} Q_{X}) - \log M(\tau)(Q_{X}) - \log M(\tau)(Q_{X}; 0) \right\} \cdot (28)$$

where $x \triangleq [x_{0}, x_{1}, \ldots, x_{\tau}]^{T}$, with $x_{a} \triangleq x_{ak}$ for $a = 0, \ldots, \tau$. So, we have seen

\begin{align}
\text{l.h.s.} \left[ 15 \right] = \lim_{h \to 0} \frac{\partial}{\partial h} T(Q_{S}, Q_{S}, Q_{X}, Q_{X}; \tau, h) \quad \text{Extr} \quad \frac{\partial}{\partial \tau} \log M(\tau)(Q_{X}; h) \quad \text{and that}\end{align}

limiting the free energy of the replicated system is defined as below

$$\mathcal{F} \triangleq -\frac{1}{K} \mathbb{E}_{y, C, H} \{ \log \mathcal{P}(y, C, H) \}$$

Recalling the fact that $\mathbb{E}(\log \Theta) = \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \mathbb{E}(\Theta^\tau)$, this free energy could be computed via

$$\mathcal{F} = -\lim_{\tau \to 0} \frac{\partial}{\partial \tau} \mathcal{F}_{\tau}$$

$$\mathcal{F}_{\tau} \triangleq \frac{1}{K} \log \mathbb{E}_{y, C, H} \{ \mathcal{P}(y, C, H) \} .$$

Following the convention of replica method like \cite{11}, we assume \cite{32} to be valid for all real-valued $\tau$ in the vicinity of $\tau = 0$, and remains valid also for integers $\tau = 1, 2, \ldots$. The rigorous mathematical minds will immediately question the validity of this last assumption. In particular, the expression obtained for integer values may not be valid for real values in general. As a matter of fact \cite{16}, the continuation of the expression to real values is not unique, e.g., $f(\tau) + \sin(\tau \pi)$ and $f(\tau)$ coincide at all integer $\tau$ for every function $f(\cdot)$. Nevertheless, as we shall see, the replica method simply takes the same expression derived for integer values of $\tau$, which is natural and straightforward in the problem at hand. The rigorous justification for the above assumption is still an open problem. Surprisingly, this continuation assumption, along with other assumptions sometimes very intricate on symmetries of solutions, leads to correct results in all non-trivial cases where the results are known through other rigorous methods, see \cite{24, 25} for examples on the AMP and GAMP cases. In other cases, the replica method produces results that match well with numerical studies.

Before proceeding to the evaluation of $\mathcal{F}$, we reformulate first the partition function $\mathcal{P}(y, C, H)$ using

$$\mathcal{P}(y, C, H) = \int_{s} \mathcal{P}(y | C, s) \int_{x} \mathcal{P}(s | H, x) \mathcal{P}(x) dx ds \quad (34)$$

$$= \int_{s} \left( \int_{u} \mathcal{P}(y | u) \delta | u - C s | du \right) dx \times$$

$$\int_{v} \left( \int_{x} \mathcal{P}(s | v) \delta | v - H x | dx \right) \mathcal{P}(x) dx \quad (35)$$

Comparing to the 1L-SLM considered in \cite{12}, our challenges here in the 2L-GLM include: first, an extra layer of network exists which suffers from mixing interference (caused by the weighting) and non-linear activation; second, an activation that is non-Gaussian distributed. To handle these, our solution is:

1) Reformulate the network as a two-fold integral in \cite{34}, so that a nested structure in the expression could be exploited to apply a “divide-and-conquer” strategy that starts backwardly from the last layer, treating previous ones as its prior.

2) Incorporate a Dirac-$\delta$ function into the non-linear activation process, see \cite{35}, so that the non-AWGN random mapping could be separated from the linear deterministic weighting, which further paves way for the essential Gaussian approximation to the activation (non-linear and non-Gaussian).

Following this line, we take 4 steps to compute the free energy.

C. Replica Analysis–Part 2: Computing the Free Energy

This subsection elaborates more details on the proof of some key steps skipped from last subsection to ease reading. These contents fit well into the framework of free energy computation for the replicated system, after noticing from \cite{22}
Step 1: Gaussian approximation for \( \mathbb{E}[P^r(y|C, H)] \) of \( \mathcal{F}_r \):

\[
\mathbb{E}_{y,C,H}[P^r(y|C, H)] = \mathbb{E}_{C,H}\left[ \mathbb{E}_y[\mathbb{P}(y|x_a, C, H) \mathbb{P}(x_a) \mathbb{d}x_a] \mathbb{d}y \right] \tag{36}
\]

Then, it holds

\[
\mathbb{E}_{y,C,H}\left\{ P^r(y|C, H) \right\} = \mathbb{E}_{C,H}\left\{ \int_y \prod_{a=0}^\tau \left( \int_{v_a} \mathbb{P}(y|v_a) \mathbb{d}v_a \right) \mathbb{P}(v_a) \mathbb{d}v_a \right\} \tag{37}
\]

where the subscript \( a \) refers to the replica number, e.g., \( x_a \) being \( a \)-th replica of \( x \), and the following definitions are used: \( X \triangleq [x_0, \ldots, x_{\tau}] \), \( U \triangleq [u_0, \ldots, u_{\tau}] \), \( S \triangleq [s_0, \ldots, s_{\tau}] \), and \( V \triangleq [v_0, \ldots, v_{\tau}] \). Moreover, the \((a, n)\)-th element of \( V \) is denoted by \( v_{an} \triangleq [C^a_{n}]_{a,n} \), while the expectation in (38) is taken over \( \mathbb{P}(S) = \mathbb{E}_X \left[ \prod_{t=0}^\tau \mathbb{P}(S|U) \mathbb{E}_H \left\{ \delta(U - HX) \right\} \right] \).

After that, this element becomes the sum of a large number of random variables. According to central limit theorem, \( v_{an} \) could be approximated by a Gaussian r.v. distributed as \( \mathcal{N}(\varnothing|0, \sum_{m=1}^M s_{am}s_{bm}/N) \) because

\[
\mathbb{E}[v_{an}] = \mathbb{E}\left[ \sum_{m=1}^M c_{nm}s_{am} \right] = 0 \tag{39}
\]

\[
\mathbb{E}[v_{an}v_{bn}] = \mathbb{E}\left[ \sum_{m=1}^M c_{nm}s_{am}\sum_{m'=1}^M c_{nm'}s_{bm'} \right] = \sum_{m=1}^M s_{am}s_{bm}/N \tag{40}
\]

Letting \( v_n \triangleq [v_{0n}, v_{1n}, \ldots, v_{\tau n}]^T \) and applying Gaussian approximation, eq. (38) could be rewritten as

\[
\mathbb{E}_{y,C,H}\left\{ P^r(y, C, H) \right\} = \mathbb{E}_S \left[ \int_y \int_{V} \mathbb{P}(y|v_a) \mathbb{P}(v_a) \mathbb{d}v_a \right] \mathbb{d}y \tag{41}
\]

Step 2: Approximation to \( \mathcal{F}_r \) as per large deviation theory:

Letting \( Q_S \triangleq \frac{1}{M} STS \), the density of \( Q_S \) could be given as

\[
\mathbb{P}(Q_S) = \mathbb{E}_S \left[ \prod_{0 \leq a \leq \delta} \mathbb{P}(M|Q_S) \mathbb{d}M \right] \sum_{m=1}^M s_{am}s_{bm} \tag{42}
\]

For this density function, there exists a correlation in \( s_a \) due to the linear weighting; fortunately, such a correlation will vanish as a consequence of the self-averaging effect in large system limit. The self-average effect suggests that, in a large system, the random vector \( u_n \) will approximately be distributed as Gaussian with a zero mean and a covariance matrix of \( \sigma_x^2 H H^T \), whose limit is \( \sigma_x^2 I \). On the other hand, the transitional distribution \( \mathbb{P}(s_a|u_a) \) is an identical and element-wise random mapping, meaning that all elements in the vector \( s_a \) are i.i.d.. Together with the fact that \( |Q_S|_{ab} = \frac{1}{M} \sum_{m=1}^M s_{am}s_{bm} \), it is natural to have the large deviation theory come into play. This large deviation theory is a branch of statistical studies that offers many useful results for the limiting distribution of the sum of i.i.d. random variables. Particularly in our case, we find that the target p.d.f. \( \mathbb{P}(Q_S) \) could be represented via the rate function \( R^{(r)}(Q_S) \)

\[
R^{(r)}(Q_S) = \sup_{Q_S} \left\{ \text{tr}(Q_S \tilde{Q}_S) - \log \mathbb{E}_S \left[ \exp \left( \text{tr}(Q_S S^T S) \right) \right] / M \right\}
\]

Based on these results, we continue to simplify (41) as

\[
\mathbb{E}_{y,C,H}\left\{ P^r(y, C, H) \right\} = \int_{Q_S} \int_{y_a} \mathbb{P}(y|v_a) \mathbb{P}(v_a) \mathbb{d}v_a \mathbb{d}y_a \mathbb{d}Q_S \tag{43}
\]

\[
\mathbb{P}(Q_S) = \mathbb{E}_S \left[ \prod_{0 \leq a \leq \delta} \mathbb{P}(M|Q_S) \mathbb{d}M \right] \sum_{m=1}^M s_{am}s_{bm} \tag{42}
\]

\[
\mathbb{P}(Q_S) = \mathbb{E}_S \left[ \prod_{0 \leq a \leq \delta} \mathbb{P}(M|Q_S) \mathbb{d}M \right] \sum_{m=1}^M s_{am}s_{bm} \tag{42}
\]

Upon this, we apply the Varadhan’s theorem \( \mathcal{F}_r \) to get the following Laplace approximation or saddle-point approximation to \( \mathcal{F}_r \), whose definition was in (44)

\[
\mathcal{F}_r = \sup_{Q_S} \left\{ \frac{N}{K} \mathcal{G}^{(r)}(Q_S) - \frac{1}{K} R^{(r)}(Q_S) \right\} \tag{45}
\]

Similar to \( v_{an} \) in (39)-(40), the element \( u_{am} \) of the matrix \( U \) could be handled in an analogous way. In particular, we define \( Q_X \triangleq \frac{1}{M} X^T X \) whose p.d.f. is then given by

\[
\mathbb{P}(Q_X) = \mathbb{E}_X \left[ \prod_{0 \leq a \leq \delta} \mathbb{P}(M|Q_X) \mathbb{d}M \right] \sum_{m=1}^M s_{am}s_{bm} \tag{42}
\]

According to \( \mathcal{F}_r \), the probability measure of \( Q_X \) satisfies the Varadhan’s theorem with a rate function \( R^{(r)}(Q_X) \), and it holds

\[
\log \mathbb{E}_S \left[ \exp \left( \text{tr}(Q_S S^T S) \right) \right] = \log \int_{S} \exp(\text{tr}(Q_S S^T S)) dS.
\]

Defining \( u_m \triangleq [u_{am}]_{a=0}^\tau \), it further breaks down as

\[
\log \mathbb{E}_S \left[ \exp \left( \cdot \right) \right] = \log \int_{Q_X} dQ \mathbb{P}(Q_X) \prod_{m=1}^M \int_{s_m} \int_{u_m} \exp \left( \frac{1}{M} \sum_{m=1}^M s_{am}s_{bm} \right) \mathbb{P}(s_m|u_m) \mathbb{N}(u_m|0, \frac{Q_X}{\alpha}) d\mathbb{u}_m d\mathbb{s}_m
\]

\[
= \log \int dQ \mathbb{P}(Q_X) \int d\mathbb{u} \exp(\text{tr}(Q_S S) \mathbb{P}(S|u)\mathbb{N}(u|0, \frac{Q_X}{\alpha})) M
\]

Finally, by denoting $x \triangleq [x_0, x_1, \ldots, x_T]^T$, we have
\[
\log \mathbb{E}_S \{ \exp (\cdot) \} = \mathbb{K} \sup_{Q_X} \left[ \alpha G^{(\tau)}(Q_S, Q_X) - R^{(\tau)}(Q_X) \right] \tag{47}
\]
\[
G^{(\tau)}(\hat{Q}_S, Q_X) \triangleq \log \int du ds \exp(s^T \hat{Q}_S s) \mathcal{P}(s|u) \mathcal{N}(u|0, \frac{Q_X}{\alpha}) \tag{48}
\]
Combining (43) and (47) yields (‘Extr’ is the extreme value)
\[
\mathcal{F} = \text{Extr}_{Q_S, Q_S, Q_X} \left[ \alpha \beta G^{(\tau)}(Q_S) - \text{tr}(Q_S Q_S) - \text{tr}(\hat{Q}_X Q_X) + \alpha G^{(\tau)}(Q_S, Q_X) + \mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\} \right] \tag{49}
\]
where the last equality uses * to differentiate an extreme point from a general (matrix) argument.

**Step 3:** Partial derivation for saddle points: By taking partial derivatives of $T(\cdot)$ w.r.t. $Q_X$, $\hat{Q}_X$, $Q_S$, and $\hat{Q}_S$, we obtain the saddle point equations below:
\[
\hat{Q}_S = \beta \frac{\partial G^{(\tau)}(Q_S)}{\partial Q_S} \tag{52a}
\]
\[
Q_S = \frac{\partial G^{(\tau)}(Q_S, Q_X)}{\partial Q_S} \tag{52b}
\]
\[
\hat{Q}_X = \alpha \frac{\partial G^{(\tau)}(Q_S, Q_X)}{\partial Q_X} \tag{52c}
\]
\[
Q_X = \frac{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \tag{52d}
\]
To further simplify the matrix derivative, we find the following identity very useful (see the supporting materials for a proof):
\[
\frac{\partial \mathcal{N}(x|a, A)}{\partial A} = -\frac{1}{2} [A^{-1} - A^{-1}(x - a)(x - a)^T A^{-1}] \mathcal{N}(x|a, A).
\]
By chain rule, this could rewrite the saddle point equations as
\[
\hat{Q}_S = \frac{\beta (Q_S^{-1} - \beta Q_S^{-1} \mathbb{E}_v [vv^T] Q_S^{-1})}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \tag{53a}
\]
\[
Q_S = \frac{\mathbb{E}_x [ss^T]}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \tag{53b}
\]
\[
\hat{Q}_X = \frac{\alpha Q_X^{-1} - \alpha Q_X^{-1} \mathbb{E}_u [uu^T] Q_X^{-1}}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \tag{53c}
\]
\[
Q_X = \frac{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \tag{53d}
\]
where the expectations are taken over the above distributions
\[
\rho_v(v) = \int_a \frac{1}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \mathbb{E}_v \{\mathcal{P}(y|v)\mathcal{N}(v|\alpha, 0, 1/4 Q_S)\} dy
\]
\[
\rho_s(s) = \frac{1}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \int_a \mathbb{E}_u \{\mathcal{P}(s|u)\mathcal{N}(u|0, \frac{Q_X}{\alpha})\} du
\]
\[
\rho_u(u) = \frac{1}{\mathbb{E}_x \left\{ \exp \left( x^T \hat{Q}_X x \right) \right\}} \int_s \mathbb{E}_v \{\mathcal{P}(s|v)\mathcal{N}(v|0, \frac{Q_X}{\alpha})\} ds
\]
$\mathcal{P}_X(x)$ being the prior density. On [53], we note that it is in general very difficult to solve a four-matrix-argument solution for the saddle point equations (53), as there are too many arguments to solve. Although exceptions do exist, e.g., in case that all the prior and the transitional probabilities follow Gaussian distributions, the MMSE estimators there are usually simple to analyze and were thus extensively studied in the literature. For instance, in the all Gaussian case above, the exact MMSE particularize as the well known linear MMSE (LMMSE) estimator, whose asymptotic performance was well captured by the Tse-Hanly equations [29]. In this context, it is usually assumed that the solution will exhibit a certain pattern in the structure of each solution matrix, which is termed replica symmetry. The replica symmetry considered here assumes that each matrix is a circular matrix consisting of two free parameters, thus reducing the number of individual equations from $4(\tau + 1)^2$ to $4 \times 2$. It is worthy of noting that assuming replica symmetry, the free energy could be obtained analytically; however, there is unfortunately no known general condition for the replica symmetry to hold [12]. The replica-symmetric solution, assumed for analytical tractability in this paper, is consistent with numerical results in the simulation sections. In next step we provide more detail on the replica symmetric solutions.

**Step 4:** Solutions under replica symmetry: Assuming replica symmetry, each solution matrix is parameterized by two free arguments, i.e., (for simplicity, we omit the superscript * despite of that fact that the variable is an extreme point, i.e., a solution to the saddle point equations)
\[
Q_X = \tau (c - d) I + d \mathbf{1} \mathbf{1}^T, \quad \hat{Q}_X = \tau (\tilde{c} - \tilde{d}) I + \tilde{d} \mathbf{1} \mathbf{1}^T \tag{54a}
\]
\[
Q_S = \tau (e - f) I + f \mathbf{1} \mathbf{1}^T, \quad \hat{Q}_S = \tau (\tilde{e} - \tilde{f}) I + \tilde{f} \mathbf{1} \mathbf{1}^T \tag{54b}
\]
with $(c, d, \tilde{c}, \tilde{d}, e, f, \tilde{e}, \tilde{f})$ being the free parameters, and $\mathbf{1} \mathbf{1}^T$ denoting a all-one matrix of the size $(\tau + 1) \times (\tau + 1)$. For [53], letting $P_1 \triangleq \mathbb{E}_u [vv^T]$ and $P_2 \triangleq \mathbb{E}_u [uu^T]$, the two matrices exhibit also some replica symmetry, so we have
\[
\rho_1 = \rho_2 \triangleq \rho \exp(\gamma g, h, p, q) \triangleq \rho \exp(\gamma g, h, p, q) \tag{55}
\]
\[
\rho_2 \triangleq \rho \exp(\gamma g, h, p, q) \tag{56}
\]
with $(g, h, p, q)$ being auxiliary parameters depending on $(c, \tilde{d}, d, e, f, \tilde{e}, \tilde{f})$. Using [50], one could rewrite the free energy as follows to emphasize explicitly its dependency on the eight parameters $(c, \tilde{d}, d, e, f, \tilde{e}, \tilde{f})$ (as well as on the individual parameter $\tau$)
\[
\mathcal{F} = -\lim_{\tau \rightarrow 0} \frac{\partial}{\partial \tau} \mathcal{F}(\tau, c, \tilde{d}, d, e, f, \tilde{e}, \tilde{f}) \tag{57}
\]
For this new expression, it is important to note that all the eight parameters of $\mathcal{F}(\tau, c, \tilde{d}, d, e, f, \tilde{e}, \tilde{f})$ are actually

Footnote 3: According to [12], the validity of replica symmetry can be checked by calculating the Hessian of at the replica symmetric supremum [39]. If the Hessian is positive definite, then the replica symmetric solution is stable against replica symmetry breaking, and it is the unique solution because of the convexity of the function. Under equal-power binary input and individually optimal detection, [13] showed that if the system parameters satisfy certain condition, the replica-symmetric solution is stable against replica symmetry breaking. In some other cases, replica symmetry can be broken [31]. Recently, Reeves and Pfister [32] proved that the replica-symmetric prediction is exact for compressed sensing with Gaussian matrices.
functions of $\tau$, as one may recall from [19] and [43] that the operations of $\text{Extr}$ and $\sup$ are carried out for a given $\tau$. In this regard, it is more precise to re-express the $\mathcal{F}_\tau$ term as $\mathcal{F}(\tau, c_0, d_0, \tilde{c}_0, \tilde{d}_0, e_0, f_0, \bar{e}, \bar{f})$. Deriving the analytical results for all these eight $\tau$-dependent parameters are in general a challenging task, and thus a typical way adopted by statistical physicists for decades is to exchange the partial derivative operation $\frac{\partial}{\partial \tau}$ outside the $\mathcal{F}_\tau$ term with the $\text{Extr}$ or $\sup$ operation inside $\mathcal{F}_\tau$. Such an exchange is non-rigorous in general sense as counter examples abound in the mathematical world, though it had obtained great empirical successes during the years. In this paper, we apply a new approach to avoid such an exchange, and this approach in itself is rigorous in mathematical sense. Our approach is

$$\mathcal{F} = - \lim_{\tau \to 0} \frac{\partial}{\partial \tau} \mathcal{F}(\tau, c_0, d_0, \tilde{c}_0, \tilde{d}_0, e_0, f_0, \bar{e}, \bar{f})$$

(58)

where the first equality uses an independent variable $\tau$ to highlight the explicit dependency, and the last equality is due to the fact given by [12]-[13] that in overall effect, the free energy $\mathcal{F}$ depends only on its eight parameters evaluated at $\tau = 0$. In other words, we don’t have to solve out the parameters’ expressions for arbitrary $\tau$ (and then perform a partial derivation followed by a limit); for the computation of free energy, we only need to solve them out at the origin point $\tau = 0$. That is, we simply set $\tau = 0$ in (53) and then solve the coupled equations obtained. Our new approach is distinct from the (non-rigorous) conventional way in that we consider here jointly three operations, $\lim_{\tau \to 0}$, $\frac{\partial}{\partial \tau}$, and $\mathcal{F}_\tau$, but in classical way, it considers the latter two only, leaving it not too many choices except interchanging the two operations.

In the followings, we apply our new approach to solve/simplify the coupled equations. For notational simplicity, we abuse $(c, d, \tilde{c}, \tilde{d}, e, f, \bar{e}, \bar{f})$ to denote $(c_0, d_0, \tilde{c}_0, \tilde{d}_0, e_0, f_0, \bar{e}, \bar{f})$, whenever their meanings are obvious from the context. The derivation is divided into four parts, detailed as below.

**Step 4.1:** To solve (53a), we first evaluate $g$ and $h$ as below

$$g = \frac{\int_y \int_v (v_0) \prod_{a=0}^2 \mathcal{P}(y|v_0) \mathcal{N}(v|0, \frac{1}{\beta} \mathcal{Q}_S) dv dy}{\int_y \int_v \prod_{a=0}^2 \mathcal{P}(y|v_0) \mathcal{N}(v|0, \frac{1}{\beta} \mathcal{Q}_S) dv dy}$$

(60)

$$h = \frac{\int_y \int_v \int_v (v_0) \prod_{a=0}^2 \mathcal{P}(y|v_0) \mathcal{N}(v|0, \frac{1}{\beta} \mathcal{Q}_S) dv dy}{\int_y \int_v \int_v \prod_{a=0}^2 \mathcal{P}(y|v_0) \mathcal{N}(v|0, \frac{1}{\beta} \mathcal{Q}_S) dv dy}$$

(61)

The key is to decouple $\mathcal{Q}_S$. Using the matrix inverse lemma, i.e., $(A + BC)^{-1} = A^{-1} - A^{-1}B(I + CA^{-1}B)^{-1}CA^{-1}$, we have $\beta \mathcal{Q}_S^{-1} = e^{-\beta} I - \frac{\beta}{\beta - f} (1 - \frac{\beta}{\beta - f}) 11^T$. Denote $A \triangleq \frac{\beta}{\beta - f}$, $B \triangleq \frac{\beta}{\beta - f} (1 - \frac{\beta}{\beta - f})$, and evaluate

$$\exp(-\frac{1}{2} v^T \beta \mathcal{Q}_S^{-1} v) = \exp \left[ -A \sum_{a=0}^2 v_a^2 + \left( \frac{\sqrt{B}}{2} \sum_{a=0}^2 v_a \right)^2 \right]$$

$$\int_y \sqrt{\frac{n}{2\pi}} \exp \left[ -A \sum_{a=0}^2 v_a^2 \right] \sum_{a=0}^2 v_a \xi \mathcal{N}(v|0, \frac{1}{\beta} \mathcal{Q}_S) dv$$

(62)

where the last equality uses the Hubbard-Stratonovich transform [33]: $\exp(x^2) = \sqrt{\frac{2\pi}{x}} \exp(-\frac{1}{2} x^2 + \sqrt{\frac{2\pi}{x}} x) dx$.

**Step 4.2:** Next calculate (53b). By the Matrix Inversion Lemma, we see $\alpha \mathcal{Q}_X^{-1} = e^{-\beta} I - \frac{\beta}{\beta - f} (1 - \frac{\beta}{\beta - f}) 11^T$. Defining

$$A' \triangleq \frac{\alpha}{c - d}, \quad B' \triangleq \frac{\alpha d}{(c - d)(c + d) \xi}$$

(71)
and applying again the Hubbard-Stratonovich transform, we decouple the tangled cross terms like \(u, u_j\) and \(s_i, s_j\) at the cost of an additional integral w.r.t. to a new auxiliary variable
\[
\exp \left( -\frac{1}{2} u^T \alpha Q X^{-1} u \right) = \sqrt{\frac{\eta}{2\pi}} \int \frac{d\xi}{\xi}
\]
\[
\exp \left( -\frac{1}{2} A' \sum_{a=0}^{\tau} (u_a)^2 \right) \sqrt{\frac{\eta}{2\pi}} \int \frac{d\xi}{\xi}
\]
\[
\exp \left( s^T \bar{Q} s \right) = \sqrt{\frac{\gamma}{2\pi}} \int \frac{d\xi}{\xi}
\]
\[
\exp \left( -\tilde{f} \sum_{a=0}^{\tau} (s_a)^2 - \frac{\gamma}{2} \xi^2 + 2\gamma \tilde{f} \sum_{a=0}^{\tau} s_a \right)
\]
With these decoupling results, \(c\) now can be evaluated (\(\tau \to 0\))
\[
\int \exp(s^T \bar{Q} s) \mathcal{P}(s|u) N(u|0, \frac{Q X}{\alpha}) du ds = C \sqrt{\frac{2\pi}{A' - B'}}
\]
\[
\int s^2 \exp(s^T \bar{Q} s) \mathcal{P}(s|u) N(u|0, \frac{Q X}{\alpha}) du ds = C' \sqrt{\frac{2\pi}{A' - B'}}
\]
\[
\int s^2 \mathcal{P}(s|u) N \left( u \left( \sqrt{\frac{B'}{A'(A' - B')}} \frac{1}{A} \right) \right) du ds d\xi
\]
where \(C' = (2\pi)^{-\frac{d}{2}} [\alpha^{-1} Q X]^{-\frac{1}{2}}\), for more detail on the proof see the supporting materials. Combining (72)-(73) yields
\[
eq \int s^2 \mathcal{P}(s|u) N \left( u \left( \sqrt{\frac{B'}{A'(A' - B')}} \frac{1}{A} \right) \right) du ds d\xi
\]
(74)
On the other hand, we have to come to the simplification of \(f\)’s numerator (at \(\tau \to 0\))
\[
\int \int s_u s_{1u} \exp(s^T \bar{Q} s) \mathcal{P}(s|u) N(u|0, \frac{Q X}{\alpha}) du ds = C' \times
\]
\[
\int \frac{2\pi}{A' - B'} \frac{s^2}{A' - B'} \left[ \frac{s_u N_{s_u|u}(\zeta, \frac{1}{2j} \sqrt{\frac{d}{2} \frac{\xi}{\alpha}, \frac{\xi}{\alpha}}) du ds}{2} \right]^2 - \frac{D}{\xi} d\xi d\zeta
\]
which, together with (72), further gives
\[
f = \int \int \int \frac{s_u N_{s_u|u}(\zeta, \frac{1}{2j} \sqrt{\frac{d}{2} \frac{\xi}{\alpha}, \frac{\xi}{\alpha}}) du ds}{2} - \frac{D}{\xi} d\xi d\zeta
\]
where \(N_{s_u|u}(a, A, b, B) \triangleq \mathcal{P}(s|u) N(s|a, A) N(u|b, B)\).

**Step 4.3:** Before simplifying \([53]\), we still need \(P_2\), and we start from the numerator of \(p\) as given in \([56]\) (when \(\tau \to 0\))
\[
\int \int s_u s_{1u} \exp(s^T \bar{Q} s) \mathcal{P}(s|u) N(u|0, \frac{Q X}{\alpha}) du ds
\]
\[
= C' \sqrt{\frac{2\pi}{A' - B'}} \frac{s^2}{A' - B'} \frac{s_u N_{s_u|u}(\zeta, \frac{1}{2j} \sqrt{\frac{d}{2} \frac{\xi}{\alpha}, \frac{\xi}{\alpha}}) du ds}{2} - \frac{D}{\xi} d\xi d\zeta
\]
(77)
Combining (77) and (72), we get
\[
p = \lim_{\tau \to 0} \frac{1}{A' - B'} = \frac{c}{\alpha}.
\]
(78)

For the simplification of \(q\), we follow a procedure similar to that of \(f\) in \([75]-[76]\), and the result is
\[
q = \frac{\int \int \int \left| \frac{s_u N_{s_u|u}(\zeta, \frac{1}{2j} \sqrt{\frac{d}{2} \frac{\xi}{\alpha}, \frac{\xi}{\alpha}}) du ds}{2} \right|^2 - \frac{D}{\xi} d\xi d\zeta}{\int \int \int \left| \frac{s_u N_{s_u|u}(\zeta, \frac{1}{2j} \sqrt{\frac{d}{2} \frac{\xi}{\alpha}, \frac{\xi}{\alpha}}) du ds}{2} \right|^2 - \frac{D}{\xi} d\xi d\zeta}
\]
\[
\frac{E}{\alpha} = \frac{\int \frac{1}{2} (E - F) - \alpha p(E - F)^2}{\int \frac{1}{2} (E - F) - \alpha p(E - F)^2}
\]
(79)

The simplification on \(\tilde{d}\) is analogous to that of \(\tilde{f}\) via the same matrix decomposition technique. Thus, we skip the detail and provide below its result:
\[
\tilde{d} = \frac{\alpha(\alpha q - d)}{2(c - d)^2}.
\]
(80)

**Step 4.4:** To establish the SISO equivalence, we recall that \(\tilde{c} = 0\), and apply the Hubbard-Stratonovich transform \([33], [35]\) to decouple a cross term arising in the simplification of \(c\) and \(d\), i.e.,
\[
\lim_{\tau \to 0} \frac{\int \frac{1}{2} y - \sqrt{\frac{2d}{\eta}}}{\int \frac{1}{2} y - \sqrt{\frac{2d}{\eta}}}
\]
\[
\int \frac{1}{2d} \mathcal{P}(x) dx dy = 1
\]
(82)

This further yields
\[
c = \mathbb{E}_x \left[ x^2_0 \exp(x^T \bar{Q} X) \right] = \int X^2 \mathcal{P}(X) dX
\]
(83)
\[
d = \mathbb{E}_x \left[ x_0 x_1 \exp(x^T \bar{Q} X) \right] = \int \langle X \rangle \mathcal{P}(Y) dY
\]
(84)

We interpret the distribution \(\mathcal{N}(y|x, \frac{1}{2j})\) in the above equation a likelihood distribution of an observation \(Y\) given the input \(X_0\) in the context of a SISO system that reads \(Y = X_0 + W\), where \(X_0 \sim \mathcal{P}_X(X_0)\), \(W \sim \mathcal{N}(W|0, \eta)\), \(\eta = \frac{1}{2d}\), and \(Y\) is the MMSE estimate of \(X_0\), i.e.,
\[
\langle X \rangle = \int X_0 \mathcal{N}(X|X_0, \frac{1}{2d}) \mathcal{P}(X_0) dX_0
\]
(85)
which establishes the SISO equivalence.

Given the solutions to the fixed point equations, i.e., \((c', d', \bar{c}', \bar{d}', c^*, \bar{c}^*, \bar{d}^*, f^*, \bar{f}^*, \tilde{f}^*)\), we are now able to obtain the free energy \(F\) by substituting these solutions back to \([54]\) and later to \([51]\), which completes the computation task.

**IV. ASYMPTOTIC ANALYSIS FOR L-LAYER CASE**

**A. Results for Exact MMSE Estimator in ML-GLM**

**Claim 2 (Joint distribution: L-layer):** For the estimation in ML-GLM illustrated as Fig. [4] the exact MMSE estimation of a MIMO nature is identical, in the joint input-and-estimate distribution sense, to a simple SISO estimation under an AWGN setting, i.e., \((k = 1, \ldots, N_1)\)
\[
(x_{0k}, \langle X_k \rangle) \doteq (X_0, \langle X \rangle),
\]
(86)
where $X_0$ and $(X)$ are similarly defined as in Claim 2 except the noise variance $\eta = 1/(2d)$ is solved from Algorithm 1.

Claim 2 indicates that, the existence of a SISO equivalence is not a sporadic phenomenon, but a universal truth that goes along with the multi-layer GLM. Such a “decoupling property” stands at the root of the replica method in statistical physics [25]. Owing to the generality of the multi-layer model, Claim 2 embraces many existing results as its special cases, including:

1) $L = 2$, GLM: Claim 1 of this paper is a natural degeneration of Claim 2 if one initializes $L$ as 2 in Algorithm 1 and makes some trivial notation changes.

2) $L = 1$, GLM [13]: In this case, the model degenerates to a (single-layer) generalized linear one, in which Schülke [13] had shown the fixed point equations of an MMSE estimation result in the GLM could be written as follows

$$d = \int \left[ \frac{\int f_z p_X(x)N(x|\frac{1}{2\alpha})dx}{f_z p_X(x)N(x|\frac{1}{2\alpha})dx} \right]^2 d\zeta$$

$$q = \int \left[ \frac{\int f_z p_Y(y|z)N(z|\frac{1}{2\alpha}, \frac{1}{\alpha})dx}{f_z p_Y(y|z)N(z|\frac{1}{2\alpha}, \frac{1}{\alpha})dx} \right]^2 D\zeta dy$$

$$\tilde{d} = \frac{\alpha(\alpha q - d)}{2(\sigma_X^2 - d)^2}$$

which agrees perfectly with Claim 2 in case of $L = 1$.

3) $L = 1$, SLM [12, 24]: The SLM is a further particularization of the GLM with $p(y|x) = N(y|x, \sigma_w^2)$. Substituting it back into the above GLM’s fixed point equations, one gets a single-formula fixed point equation:

$$\eta = \sigma_w^2 + \frac{1}{\alpha} \xi(\eta),$$

where $\xi(\eta)$ (as stated before) represents the average MSE of the AWGN channel, $Y = X + W$, with $X \sim p_X(x)$ and $W$ having a zero mean and a variance of $\eta$. This result was previously reported by [12] in the context of CDMA multiuser detection, and by [24] in the context of state evolution of AMP, another renowned statistical inference algorithm.

### B. Sketch of Proof

Similar to Sec. III-A, we will prove this moment identity:

$$\mathbb{E}_{y_{0:k}, y_{H^{(o)}}} \left[ x_{0:k}^T y_{k}\right] = \mathbb{E}_{y_{0},y} \left[ X_{0}^T(X)\right]$$

First of all, we notice that the discussions in Sec. III-B are indeed applicable to arbitrary $L$, so, for $L > 2$, we only need to revisit its free energy computation. To this end, we start all over again from the last layer and trace backward repeatedly until its very first, treating all previous layers as a prior to the current one. It begins with

$$F = \frac{1}{2} \lim_{T \to \infty} \frac{\partial}{\partial T} \log \mathbb{E}_{y_{H^{(o)}}} \left[ Z^{(T)}(y, H^{(o)}) \right]$$

where $Z(y, H^{(o)}) = p(y|x^o)$ is the partition function in the ML-GLM setting, and the expectation further expands

$$\mathbb{E}_{y_{0:k}, y_{H^{(o)}}} \left[ Z^{(T)}(y, H^{(o)}) \right] = \mathbb{E}_{y_{1:k}} \left[ Z^{(T)}(y_{0:k}, H^{(o)}) \right]$$

where $Z^{(T)}(y_{0:k}, H^{(o)})$ denotes the $a$-th replica in the $L$-th layer (i.e., the last). We also have $p(X^{(1)}) = p(X)$, and for $\ell = L, \cdots, 2$,

$$p(X^{(\ell)}) = \mathbb{E}_{H^{(\ell-1)}} \left[ \int Z^{(\ell-1)} p(X^{(\ell)}|Z^{(\ell-1)}) \right]$$

$$\mathbb{E}_{H^{(\ell-1)}} \left[ \delta(Z^{(\ell-1)} - H^{(\ell-1)}X^{(\ell-1)}) \right]$$

Algorithm 1: Fixed Point Equations of MMSE Estimator

$$p^{(\ell)}(x|z) \triangleq \frac{p^{(\ell)}(x|z)}{p^{(\ell)}(x|z)}, \quad N^{(\ell)}(\cdot) \triangleq N^{(\ell)}(\cdot)$$

for $\ell = 1, \cdots, L$

$$T^{(\ell)}_X \triangleq \begin{cases} \ell = 1 : \sigma_X^2 \\ \ell > 1 : \int [x] p^{(\ell)}(x|z) N(z|0, \frac{T^{(\ell-1)}}{\alpha \tau_{\ell-1}}) dz dx \end{cases}$$

end

for $\ell = L, \cdots, 1$

$$q^{(\ell)} = \begin{cases} \ell = L : \int \frac{f \cdot p^{(L)}(y|x)N(z|\frac{1}{2\alpha}, \frac{1}{\alpha})dx}{f \cdot p^{(L)}(y|x)N(z|\frac{1}{2\alpha}, \frac{1}{\alpha})dx} D\zeta dy \\ \ell < L : \int \frac{f \cdot N^{(\ell)}(z|\frac{1}{2\alpha}, \frac{1}{\alpha})dy}{f \cdot N^{(\ell)}(z|\frac{1}{2\alpha}, \frac{1}{\alpha})dy} D\zeta dz dx \end{cases}$$

$$\tilde{d}^{(\ell)} = \frac{\alpha(\alpha q^{(\ell)} - d^{(\ell)})}{2(T^{(\ell)}_X - d^{(\ell)})^2}$$

end

for $\ell = 1, \cdots, L$

$$d^{(\ell)} = \begin{cases} \ell = 1 : \int f \cdot p_X(x)N(x|\frac{1}{2\alpha})dx d\zeta \\ \ell > 1 : \int f \cdot N^{(\ell)}(z|\frac{1}{2\alpha}, \frac{1}{\alpha})dy dx \end{cases}$$

$$D\zeta dx$$

end

where $Z(y, H^{(o)}) = p(y|x) = \mathbb{P}(y|x)$ is the partition function in the ML-GLM setting, and the expectation further expands

$$\mathbb{E}_{y_{0:k}, y_{H^{(o)}}} \left[ Z^{(T)}(y, H^{(o)}) \right] = \mathbb{E}_{y_{1:k}} \left[ Z^{(T)}(y_{0:k}, H^{(o)}) \right]$$

where $Z^{(T)}(y_{0:k}, H^{(o)})$ denotes the $a$-th replica in the $L$-th layer (i.e., the last). We also have $p(X^{(1)}) = p(X)$, and for $\ell = L, \cdots, 2$,
The augmented matrix representation for complex-valued case.

Next, we handle (90) and (91) in an analogous way to (39), respectively. Then, the following saddle-point equations could be obtained ($\ell = L$, $\cdots$, 1)

$$
\hat{Q}_X^{(\ell)} = -\frac{\alpha_{\ell}}{2} \left[ (Q_X^{(\ell)})^{-1} - \alpha_{\ell} [Q_X^{(\ell)}]^{-1} \right] \left( z^{(\ell)} [z^{(\ell)}]^T \right) [Q_X^{(\ell)}]^{-1} 
$$

$$
Q_X = E_{x_n} \left( x^{(\ell)} [x^{(\ell)}]^T \right) 
$$

with the expectations being taken over

$$
P(z^{(\ell)}) = \frac{\int \exp \left( x^{(\ell)} + 1 \right) P(x) P(z) N(z) \mid 0, \frac{1}{\alpha_{\ell}} Q_X^{(\ell)} \right) dx}{\int \exp \left( x^{(\ell)} Q_X^{(\ell)} x \right) P(x) N(z) \mid 0, Q_X^{(\ell-1)} \alpha_{\ell-1} \right) dx} 
$$

and

$$
P(x^{(\ell)}) = \frac{\int \exp \left( x^{(\ell)} Q_X^{(\ell)} x \right) P(x) N(z) \mid 0, Q_X^{(\ell-1)} \alpha_{\ell-1} \right) dx}{\int \exp \left( \frac{x^{(\ell)}}{Q_X^{(\ell)} x} \right) P(x) N(z) \mid 0, Q_X^{(\ell-1)} \alpha_{\ell-1} \right) dx} 
$$

where $Q_X^{(L+1)} = O$, and $Q_X^{(0)} = E_{x_n} \left\{ x x^T \exp(x^T Q_X x) \right\}$.

After that, assuming the solutions to the saddle-point equations exhibits the so-called replica symmetry, we compute the following items one by one: first, (92a) using Step 4.1 as $\ell = L$ and using Step 4.3 as $\ell < L$; then, (92b) using Step 4.2 as $\ell > 1$ and Step 4.4 as $\ell = 1$.

Finally, we get the fixed-point equations of Algo. 1 after some algebraic manipulations.

C. Extension to Complex-Valued Settings

Until now the discussion has been based on a real-valued setting of the ML-GLM system, in which both the inputs and the transform matrix take real values. In practice, particularly in wireless communication systems like 5G, spectral efficiency is a major concern, and the transmission is usually designed to be complex. In this section, we consider the extension of previous analysis to the complex settings. We follow [12, Sec. V] to divide our discussion into 4 different cases: (a) real-input, real-transform; (b) complex-input, real-transform; (c) real-input, complex-transform; (d) complex-input, complex-transform. Since case (a) has already been studied in previous sections, we start from the second one.

In case (b), the inputs take complex values but the transform matrix is still real-valued. In this case, the system can be regarded as two uses of the real-valued transformations, where the inputs and the two transformations may be dependent. Since independent inputs maximize the channel capacity, there is little reason to transmit dependent signals in the two subsystems. Thus, the analysis of the real-valued transform matrices in previous sections also applies to the case of independent in-phase and quadrature components, while the only change is that the spectral efficiency is the sum of that of the two sub-systems [12, Sec. V].

In case (c), the inputs take real values, while the transform matrix is complex. Comparing the complex-valued transformation to the real-valued one, it is easy to see that the complex-valued setting is equivalent to transmitting the same real-valued input twice over the two component real-valued channels. In other words, it is equivalent to having a real-valued channel with the load halved but input power doubled, in which our previous analysis is still applicable [12, Sec. V].

In case (d), both the input and the transform matrix are complex-valued. The system model in this case could still be rewritten into an all real-valued one using the relationship between real and complex representations. We depict this new model in Fig. 3 where complex signals are reexpressed as real vectors/matrices and then mapped via the equivalent real-valued transformation. It appears that the previous analysis is not applicable to this new model as the transformation matrices here are not i.i.d. in their elements. However, as pointed out by [12, Sec. V], a closer look into the case, one would find that it is still possible to reuse the previous analysis after certain modifications. A key point here is that the variables $u$ and $v$ as defined around (9) have asymptotically independent real and imaginary components. Such an independency allows $G^{(\tau)}(Q_S, Q_X)$ and $G^{(\tau)}(Q_S)$ to be evaluated in analogy to the previous analysis. It turns out that these two terms are doubled, comparing to the previous analysis. We also notice that if we assume the same signal power for both the real and the complex settings, then the real and the imaginary components in the complex case will both see a one-half power reduction which later balances out the doubling in $G^{(\tau)}(Q_S, Q_X)$ and $G^{(\tau)}(Q_S)$ and leads to the final conclusion: Given the same signal power, Claim 2 is applicable to both the real and the complex ML-GLM's.

V. Conclusions

In this two-part work, we considered the problem of MMSE estimation for a high dimensional random input under the ML-GLM. As Part I of the two, this paper analyzed the asymptotic behavior of an exact MMSE estimator through the use of replica method. The replica analysis revealed that: 1) in terms of joint input-and-estimate distribution, the original estimation problem of MIMO nature was identical to that of a simple SISO estimation problem facing no self-interference (caused by the linear weighting), no nonlinear distortion, (caused by the random mapping), but only an effective AWGN; 2) the noise level of the above AWGN could be further determined by solving a set of coupled equations, whose dependency on the linear weighting and the random mapping was given explicitly; 3) as a byproduct of the replica analysis, the average MSE of the exact MMSE estimator could be computed directly from the fixed-point results (with no need for Monte Carlo simulations). Comparing to existing works in the literature, this paper established a decoupling principle that not only

This is different from [12, Sec. V], where the signal power in the complex setting was doubled, and the situation for $G$ there was similar.
extended the seminal work of [12] from 1L-SLM to ML-GLM, but also indicated the universal existence of the principle in estimation under different models. As later shown in Part II, this decoupling principle carries great practicality and finds convenient uses in finite-size systems. To sum up, it opens a new avenue for the understanding and justification of the ML-GLM model, which is closely related to deep learning, or more precisely, to deep inference models such as the variational auto-encoder (VAE) [8].

Replica method is not yet a rigorous method, and its justification is still an open problem in mathematical physics [12]. However, the method has evolved during the past 30 years into a extremely powerful tool for attacking complicated theoretical problems as diverse as spin glasses, wireless communications, compressed sensing, protein folding, vortices in superconductors, and combinatorial optimization [36]. Several of its important predictions have been confirmed by other rigorous approaches, e.g., the replica predictions for the SLM problem in [12] were verified in [24] using a conditioning technique, and that for the GLM case [13] was very recently confirmed by [25] through an interpolation approach. In this context, we referred to main results of this paper as claims and reminded the readers that their mathematical rigor are still pending on more breakthroughs.

Also, considering the implementation difficulty of an exact MMSE estimator, we continue to propose in Part II an approximate solution, whose computational complexity (per iteration) is as low as the GAMP, while its MSE performance is asymptotically Bayes-optimal.

VI. ACKNOWLEDGEMENT

This work was supported in part by the Scientific Research Fund of Guangzhou 201904010297, Natural Scientific Fund of Guangdong 2016A030313705, Special Fund for Applied Science and Technology of Guangdong 2015B010129001, and Natural Scientific Fund of Guangxi 2018GXNSFDA281013.

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