Abstract—We consider the problem of inferring the input and hidden variables of a stochastic multi-layer neural network from an observation of the output. The hidden variables in each layer are represented as matrices. This problem applies to signal recovery via deep generative prior models, multi-task and mixed regression, and learning certain classes of two-layer neural networks. A unified approximation algorithm for both MAP and MMSE inference is proposed by extending a recently-developed Multi-Layer Vector Approximate Message Passing (ML-VAMP) algorithm to handle matrix-valued unknowns. It is shown that the performance of the proposed Multi-Layer Matrix VAMP (ML-Mat-VAMP) algorithm can be exactly predicted in a certain random large-system limit, where the dimensions $N \times d$ of the unknown quantities grow as $N \to \infty$ with $d$ fixed. In the two-layer neural-network learning problem, this scaling corresponds to the case where the number of input features and training samples grow to infinity but the number of hidden nodes stays fixed. The analysis enables a precise prediction of the parameter and test error of the learning.

I. INTRODUCTION

Consider an $L$-layer stochastic neural network given by
\begin{align}
Z_0^\ell &= W_\ell Z_{\ell-1}^0 + B_\ell + \Xi_\ell^0, \quad \ell = 1, 3, \ldots, L-1, \\
Z_0^\ell &= \phi_\ell(Z_{\ell-1}^0, \Xi_\ell^0), \quad \ell = 2, 4, \ldots, L, 
\end{align}

where, for $\ell = 0, 1, \ldots, L$, we have true activations $Z_0^\ell \in \mathbb{R}^{n_\ell \times d}$, weights $W_\ell \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$, biases $B_\ell \in \mathbb{R}^{n_\ell \times d}$, and true noise realizations $\Xi_\ell^0$. The activation functions $\phi_\ell$ are known, non-linear functions acting row-wise on their inputs. See Fig. 1 (TOP). We use the superscript $0$ in $Z_0^\ell$ to indicate the true values of the variables, in contrast to estimated values discussed later. We model the true values $Z_0^\ell$ as a realization of random $Z_0$, where the rows $Z_{0,i}^\ell$ of $Z_0$ are i.i.d. with distribution $p_0$:
\begin{equation}
\tag{2}
p(Z_0) = \prod_{i=1}^{n_0} p_0(z_{0,i}).
\end{equation}

Similarly, we also assume that $\Xi_0^\ell$ are realizations of random $\Xi_\ell$ with i.i.d. rows $\xi_{\ell,i}^\ell$. For odd $\ell$, the rows $\xi_{\ell,i}^\ell$ are zero-mean multivariate Gaussian with covariance $N_{\ell-1}^{-1} \in \mathbb{R}^{d \times d}$, whereas for even $\ell$, the rows $\xi_{\ell,i}^\ell$ can be arbitrarily distributed but i.i.d.

Denoting by $Y := Z_L^0 \in \mathbb{R}^{n_L \times d}$ the output of the network, we consider the following matrix inference problem:
\begin{equation}
\tag{3}
\text{Estimate } Z := \{Z_\ell\}_{\ell=0}^{L-1} \text{ given } Y = Z_L^0 {\\text{ and } } \{W_{2k-1}, B_{2k-1}, \phi_{2k}\}_{k=1}^{L/2}.
\end{equation}

This inference problem arises in reconstruction with deep generative priors [1], [2]: A deep neural network is trained as a generative model for some complex data, such as an image. The generative model could be a variational auto-encoder (VAE) [3], [4], generative adversarial network (GAN) [5], [6], or deep image prior (DIP) [7], [8]. The generative model is driven by some noise-like innovations signal $Z_0^0$. Subsequent layers are then appended to model a lossy measurement process such as blurring, occlusion, or noise, resulting in a corrupted output $Y$. With the addition of the measurement layer(s), the original image or data manifests as one of the hidden variables in the network. The problem of estimating the original image from the output $Y$ is then equivalent to the inference problem (3) of estimating the values of a hidden layer in a multi-layer network from its output. Note that, in this application, the problem is not the “learning problem” for the network, since the weights and biases of the network are assumed known (i.e., trained).

In many applications, the network (1) has no noise $\Xi_\ell$ for all layers except the final one, $\ell = L$. In this case, the $Z_L^0 = g(Z_0^L)$ for some deterministic function $g(\cdot)$ representing the action of the first $L-1$ layers. Inference can then be conducted via a minimization of the form,
\begin{equation}
\tag{4}
\hat{Z}_0 := \arg \min_{Z_0} H_L(Y, Z_{L-1}) + H_0(Z_0),
\end{equation}

where $Z_{L-1} = g(Z_0)$ is the network output, the term $H_L(Y, Z_{L-1})$ penalizes the prediction error and $H_0(Z_0)$ is an (optional) regularizer on the network input. For maximum a priori (MAP) estimation one takes,
\begin{align}
\tag{5a}
H_L(Y, Z_{L-1}) &= - \log p(Y | Z_{L-1}), \\
\tag{5b}
H_0(Z_0) &= - \log p(Z_0),
\end{align}

where the output probability $p(Y | Z_{L-1})$ is defined from the last layer of model (1b): $Y = Z_L = \phi_L(Z_{L-1}, \Xi_L)$. The minimization (4) can then be solved using a gradient-based method. Encouraging results in image reconstruction have been demonstrated in [1], [2], [9]–[13]. Markov-chain Monte Carlo (MCMC) algorithms and Langevin diffusion [14], [15] could also be employed for more complex inference tasks. However, rigorous analysis of these methods is difficult due to the non-convex nature of the optimization problem. To address this issue, recent works [16]–[18] have extended Approximate Message Passing (AMP) methods to provide inference algorithms for the multi-layer networks. AMP was originally developed in [19]–[21] for compressed sensing. Similar to other AMP-type results, the performance of multi-
layer AMP-based inference can be precisely characterized in certain high-dimensional random instances. In addition, the mean-squared error for inference of the algorithms match predictions for the Bayes-optimal inference predicted by various techniques from statistical physics [22]–[24]. Thus, AMP-based multi-layer inference provides a computationally tractable estimation framework with precise performance guarantees and testable conditions for optimality in certain high-dimensional random settings.

Prior multi-layer AMP works [16]–[18], [25] have considered the case of vector-valued quantities with $d = 1$. The main contribution of this paper is to consider the matrix-valued case when $d > 1$. As we will see in Section II, the matrix-valued case applies to multi-task and mixed regression problems, sketched clustering, as well as learning certain classes of two layer networks.

To handle the case when $d > 1$, we extend the Multi-Layer Vector Approximate Message Passing (ML-VAMP) algorithm of [17], [18] to the matrix case. The ML-VAMP method is based on VAMP method of [26], which is closely related to expectation propagation (EP) [27], [28], expectation-consistent approximate inference (EC) [29], [30], S-AMP [31], and orthogonal AMP [32]. We will use “ML-Mat-VAMP” when referring to the matrix extension of ML-VAMP.

Similar to the case of ML-VAMP, we analyze ML-Mat-VAMP in a large system limit, where $n_{\ell} \to \infty$ and $d$ is fixed, under rotationally invariant random weight matrices $W_{\ell}$. In this large system limit, we prove that the mean-squared error (MSE) of the estimates of ML-Mat-VAMP can be exactly predicted by a deterministic set of equations called the state evolution (SE). In the case of ML-VAMP, the SE equations involve scalar quantities and $2 \times 2$ matrices. For ML-Mat-VAMP, the SE equations involve $d \times d$ and $2d \times 2d$ matrices. For learning problems, we will see that the SE equations enables predictions of the parameter error as well as test error.

**Notation:** Boldface uppercase letters $X$ denote matrices. $X_{n}$ refers to the $n$th row of $X$. Random vectors are row-vectors. For a function $f : R^{1 \times m} \to R^{1 \times n}$, its row-wise extension is represented by $f : R^{N \times m} \to R^{N \times n}$, i.e., $[f(X)]_{n} = f(X_{n})$. We denote the Jacobian of $f$ by $\partial f(x, y) \in R^{m \times n}$, so that $\frac{\partial f(x, y)}{\partial x}_{ij} = \frac{\partial f_{j}(x, y)}{\partial x_{i}}$. For its row-wise extension $f$, we denote by $\langle \frac{\partial f_{ij}(X, Y)}{\partial x_{i}} \rangle$ the average Jacobian, i.e., $\frac{1}{N} \sum_{n=1}^{N} \frac{\partial f}{\partial x_{i}}(X_{n}; Y_{n})$.

II. Example Applications

A. Multi-task and Mixed Regression Problems

A simple application of the matrix-valued multi-layer inference problem (3) is for multi-task regression [33]. Consider a linear model of the form,

$$Y = X F + \Xi,$$

where $Y \in R^{N \times d}$ is a matrix of measured responses, $X \in R^{N \times p}$ is a known matrix, $F \in R^{p \times d}$ are set regression coefficients to be estimated, and $\Xi$ is additive noise. The problem can be considered as $d$ separate linear regression problems – one for each column. However, in some applications, these design “tasks” are related in such a way that it benefits to jointly estimate the predictors. To do this, it is common to solve an optimization problem of the form

$$\arg \min_{F} \left\{ \frac{1}{d} \sum_{j=1}^{d} \sum_{i=1}^{N} L(y_{ij}, X F)_{ij} + \lambda \sum_{k=1}^{p} \rho(F_{k}) \right\},$$

where $L(\cdot)$ is a loss function, and $\rho(\cdot)$ is a regularizer that acts on the rows of $F_{k}$ of $F$ to couple the prediction coefficients across tasks. For example, the multi-task LASSO [33] uses loss $L(y, z) = (y - z)^{2}$ and regularization $\rho(F_{k}) = \|F_{k}\|_{2}$ to enforce row-sparsity in $F$. In the compressive-sensing context, multi-task regression is known as the “multiple measurement vector” (MMV) problem, with applications in MEG reconstruction [34], DoA estimation [35], and parallel MRI [36]. An AMP approach to the MMV problem was developed in [37]. The multi-task model (6) can be immediately written as a multi-layer network (1) by setting:

$$Z_{0} := F, \quad W_{0} := X, \quad Z_{1} := W_{0} Z_{0} = X F, \quad Y = Z_{2} := Z_{1} + \Xi.$$

Also, by appropriately setting the prior $\rho(Z_{0})$, the multi-layer matrix MAP inference (5) will match the multi-task optimization (7).
In (7), the regularization couples the columns of \( F \) but the loss term does not. In \textit{mixed regression} problems, the loss couples the columns of \( F \). For example, consider designing predictors \( F = [f_1, f_2] \) for \textit{mixed linear regression} [38], i.e.,

\[
y_i = q_i x_i^T f_1 + (1 - q_i)x_i^T f_2 + v_i, \quad q_i \in \{0, 1\},
\]

where \( i = 1, \ldots, N \) and the \( i \)th response comes from one of two linear models, but which model is not known. This setting can be modeled by a different output mapping: As before, set \( Z_1 = X F \) and let the noise in the output layer be \( \Xi = [q, v] \) which includes the additive noise \( v_i \) in (8) and the random selection variable \( q_i \). Then, we can write (8) via an appropriate function, \( y = \phi_1(Z_1, \Xi) \).

### B. Sketched Clustering

A related problem arises in \textit{sketched clustering} [39], where a massive dataset is nonlinearly compressed down to a short vector \( y \in \mathbb{R}^n \), from which cluster centroids \( f_k \in \mathbb{R}^p \), for \( k = 1, \ldots, d \), are then extracted. This problem can be approached via the optimization [40]

\[
\min_{\alpha \geq 0} \min_F \sum_{i=1}^n \left| y_i - \sum_{j=1}^d \alpha_j e^{\gamma X_i^T f_j} \right|^2,
\]

where \( X_i \in \mathbb{R}^p \) are known i.i.d. Gaussian vectors. An AMP approach to sketched clustering was developed in [41]. For known \( \alpha \), the minimization corresponds to MAP estimation with the multi-layer network model with \( Z_0 = F \), \( W_1 = X \), \( Z_1 = X F \) and using the output mapping,

\[
\phi_1(Z_1, \Xi) := \sum_{j=1}^d \alpha_j e^{\gamma X_i^T f_j} + \Xi
\]

where the exponential is applied elementwise and \( \Xi \) is i.i.d. Gaussian. The mapping \( \phi_1 \) operates row-wise on \( Z_1 \) and \( \Xi \).

### C. Learning the Input Layer of a Two-Layer Neural Network

The matrix inference problem (3) can also be applied to learning the input layer weights in a two-layer neural network (NN). Let \( X \in \mathbb{R}^{N \times N_{in}} \) and \( Y \in \mathbb{R}^{N \times N_{out}} \) be training data corresponding to \( N \) data samples. Consider the two-layer NN model,

\[
Y = \sigma(X F_1) F_2 + \Xi,
\]

with weight matrices \( (F_1, F_2) \), componentwise activation function \( \sigma(\cdot) \), and noise \( \Xi \). In (10), the bias terms are omitted for simplicity. We used the notation \( F_1 \) for the weights, instead of the standard notation \( \mathbf{W}_1 \), to avoid confusion when (10) is mapped to the multi-layer inference network (3). Now, our critical assumption is that the weights in the second layer, \( F_2 \), are known. The goal is to learn only the weights of the first layer, \( F_1 \), which are selected from a dataset of \( N \) samples \((X, Y)\).

If the activation is ReLU, i.e., \( \sigma(H) = \max\{H, 0\} \) and \( Y \) has a single column (i.e. scalar output per sample), and \( F_2 \) has all positive entries, we can w.l.o.g. treat the weights \( F_2 \) as fixed, since they can always be absorbed into the weights \( F_1 \).

In this case, \( y \) and \( F_2 \) are vectors and we can write the \( i \)th entry of \( y \) as

\[
y_i = \sum_{j=1}^d F_{2j} \sigma([X F_1]_{ij}) + \xi_i = \sum_{j=1}^d \sigma([X F_1]_{ij} F_{2j}) + \xi_i
\]

Thus, we can assume w.l.o.g. that \( F_2 \) is all ones. The parameterization (11) is sometimes referred to as the \textit{committee machine} [42]. The committee machine has been recently studied by AMP methods [43] and mean-field methods [44] as a way to understand the dynamics of learning.

To pose the two-layer learning problem as multi-layer inference, define

\[
Z_0 := F_1, \quad W_1 := X, \quad Z_1 := X F_1 \quad \Xi_2 := \Xi,
\]

then \( Y = Z_2 \), where \( Z_2 \) is the output of a 2-layer inference network of the form in (1):

\[
Y = Z_2 = \phi_2(Z_1, \Xi_2) := \sigma(Z_1) F_2 + \Xi_2.
\]

Note that \( W_1 \) is known. Also, since we have assumed that \( F_2 \) is known, the function \( \phi_2 \) is known. Finally, the function \( \phi_2 \) is row-wise separable on both inputs. Thus, the problem of learning the input weights \( F_1 \) is equivalent to learning the input \( Z_0 \) of the network (12).

### III. MULTI-LAYER MATRIX VAMP

#### A. MAP and MMSE inference

Observe that the equations (1) define a Markov chain over these signals and thus the posterior \( p(Z|Z_L) \) factorizes as

\[
p(Z|Z_L) \propto p(Z_0) \prod_{\ell=1}^{L-1} p(Z_\ell|Z_{\ell-1}) p(Y|Z_{L-1}).
\]

where the transition probabilities \( p(Z_\ell|Z_{\ell-1}) \) are implicitly defined in equation (1) and depend on the statistics of noise terms \( \Xi_\ell \). We consider both maximum a \textit{posteriori} (MAP) and minimum mean squared error (MMSE) estimation for this posterior:

\[
\hat{Z}_{\text{map}} = \arg\max_Z p(Z|Z_L)
\]

\[
\hat{Z}_{\text{mmse}} = \mathbb{E}[Z|Z_L] = \int Z p(Z|Z_L) dZ.
\]

#### B. Algorithm Details

The ML-Mat-VAMP for approximately computing the MAP and MMSE estimates is similar to the ML-VAMP method in [17], [45]. The specific iterations of ML-Mat-VAMP algorithm are shown in Algorithm 1. The algorithm produces estimates by a sequence of forward and backward pass updates denoted by superscripts \( \dagger \) and \( \dagger \) respectively.

The estimates \( \hat{Z}_\ell^\dagger \) are constructed by solving sequential problems \( Z = \{Z_\ell\}_{\ell=1}^L \) into a sequence of smaller problems each involving estimation of a single activation or preactivation \( Z_\ell \) via estimation functions \( \{G_\ell^\dagger(\cdot)\}_{\ell=1}^L \) which are selected depending on whether one is interested in MAP or MMSE estimation.
To describe the estimation functions, we use the notation that, for a positive definite matrix $\Gamma$, its Cholesky decomposition is $\Lambda_\Gamma = \Lambda_\Gamma^+ \Lambda_\Gamma^-$, where $\Lambda_\Gamma^+$ is the upper triangular matrix and $\Lambda_\Gamma^-$ is the lower triangular matrix. For $\ell = 1, \ldots, L - 1$ define the approximate belief functions:

$$b_\ell(Z_{l-1}, R_{l-1}, R_{l-1}^+, \Gamma_{l-1}^+)^2) \propto p(Z_{l-1})$$
$$= e^{-\frac{1}{2}||Z_{l-1} - Z_{l-1}^-||^2_{\Gamma_{l-1}^-} - \frac{1}{2}||Z_{l-1} - R_{l-1}^+||^2_{\Gamma_{l-1}^+} - \frac{1}{2}||Z_{l-1} - R_{l-1}^-||^2_{\Gamma_{l-1}^-}}$$

Define $b_0(Z_0|Z_{0}, \Gamma_0^+)$ and $b_L(Z_{L-1}|R_{L-1}^+, \Gamma_{L-1}^-)$ similarly.

The MAP and MMSE estimation functions are then given by the MAP and MMSE estimates for these belief densities,

$$G_{l,\text{map}} = (Z_{l}^+, \tilde{Z}_{l-1})_{\text{map}} = \argmax b_\ell(Z_{l}, \tilde{Z}_{l-1})$$

$$G_{l,\text{mmse}} = (\tilde{Z}_{l}^+, \tilde{Z}_{l-1})_{\text{mmse}} = \mathbb{E}((Z_{l}, \tilde{Z}_{l-1})|b_\ell)$$

where the expectation is with respect to the normalized density proportional to $b_\ell$. Thus, the ML-Mat-VAMP algorithm reduces the joint estimation of the vectors $(Z_0, \ldots, Z_{L-1})$ to a sequence of simpler estimations on sub-problems with terms $(Z_{l-1}, Z_{l})$. We refer to these subproblems as denoisers and denote their solutions by $G_\ell^\pm$, so that $\tilde{Z}_l^+ = G_\ell^+$ and $\tilde{Z}_{l-1}^+ = G_{l-1}^+$ corresponding to lines 9 and 21 of Algorithm 1. The denoisers $G_{l,\text{map}}^+$ and $G_{l,\text{mmse}}^+$, which provide updates to $\tilde{Z}_{l}^+$ and $\tilde{Z}_{l-1}^+$, are defined in a similar manner via $b_0$ and $b_L$ respectively.

The estimation functions (16) can be easily computed for the multi-layer matrix network. An important characteristic of these estimators is that they can be computed using maps which are row-wise separable over their inputs and hence are easily parallelizable. To simplify notation, we denote the precision parameters for denoisers $G_{l,\text{map}}^+$ in the $k$th iteration by

$$\Theta_{k,l}^+ := (\Gamma_{k,l}^+, \Gamma_{k,l-1}^-),$$
$$\Theta_{k,0}^+ := (\Gamma_{k,0}^+, \Gamma_{k-1,l}^-),$$
$$\Theta_{k,L}^+ := (\Gamma_{k,L}^+, \Gamma_{k-1,L}^-).$$

1) Non-linear layers: For $\ell$ even, since the rows of $\mathbf{Z}_\ell$ are i.i.d., the belief density $b_\ell(Z_{\ell}, \tilde{Z}_{\ell-1})$ from (15) factors as a product across rows.

$$b_{\ell}(Z_{\ell}, \tilde{Z}_{\ell-1}) = \prod_{n} b_{\ell}([Z_\ell]_{n:}, [\tilde{Z}_{\ell-1}]_{n:})$$

Thus, the MAP and MMSE estimates (16) can be performed over $d$-dimensional variables where $d$ is the number of entries in each row. There is no joint estimation across the different $n_\ell$ rows.

2) Linear layers: When $\ell$ is odd, the density $b_\ell(Z_{\ell}, \tilde{Z}_{\ell-1})$ in (15) is a Gaussian. Hence, the MAP and MMSE estimates agree and can be computed via least squares.

Although for linear layers $(G_{l,\text{map}}^+, G_{l,\text{mmse}}^+)(R_{l}^+, R_{l-1}^+, \Theta_\ell)$ is not row-wise separable over $(R_{l}^+, R_{l-1}^+)$, it can be computed using another row-wise denoiser $(\tilde{G}_{l,\text{map}}^+, \tilde{G}_{l,\text{mmse}}^+)$ via the SVD of the weight matrix $W_\ell = V_\ell \text{diag}(S_\ell) V_\ell^T$ as follows. Note that the SVD is only needed to be performed once:

$$[G_{l,\text{map}}^+, G_{l,\text{mmse}}^+] = \max_{Z_{\ell}, \tilde{Z}_{\ell-1}} \|Z_{\ell} - W_\ell Z_{\ell-1} - B_\ell\|_N^2 + \|Z_{\ell} - R_\ell^+\|_{G_{l,\text{map}}^+}^2$$

$$= \max_{Z_{\ell}, \tilde{Z}_{\ell-1}} \|V_\ell^T Z_{\ell} - \text{diag}(S_\ell) V_\ell Z_{\ell-1} - V_\ell^T B_\ell\|_N^2$$

where (a) follows from the rotational invariance of the norm, and (b) follows from the definition of denoiser $(\tilde{G}_{l,\text{map}}^+, \tilde{G}_{l,\text{mmse}}^+)(R_{l}^+, \tilde{R}_{l-1}^+, \Theta_\ell)$ given below

$$[G_{l,\text{map}}^+, G_{l,\text{mmse}}^+] := \max_{Z_\ell, \tilde{Z}_{\ell-1}} \|Z_\ell - \text{diag}(S_\ell) Z_{\ell-1} - \tilde{B}_\ell\|_N^2$$

$$= \|Z_{\ell} - \tilde{R}_{\ell}^-\|_{G_{l,\text{map}}^+}^2 + \|Z_{\ell-1} - \tilde{R}_{\ell-1}^+\|_N^2$$

Note that the optimization problem in (18) is decomposable across the rows of variables $Z_{\ell}$ and $\tilde{Z}_{\ell-1}$, and hence $[G_{l,\text{map}}^+, G_{l,\text{mmse}}^+]$ operates row-wise on its inputs.
A. Large System Limit

We follow the analysis framework of the ML-VAMP work [17], [45], which is itself based on the original AMP analysis in [21]. This analysis is based on considering the asymptotics of certain large random problem instances. Specifically, we consider a sequence of problems (1) indexed by N such that for each problem the dimensions n(N) are growing so that \( \lim_{N \to \infty} \frac{n(N)}{N} = \beta \in (0, \infty) \) are scalar constants. Note that d is finite and does not grow with N.

1) Distributions of weight matrices: For \( \ell = 1, 3, \ldots, L - 1 \), we assume that the weight matrices \( W_\ell \) are generated via the singular value decomposition,

\[
W_\ell = V_\ell \text{diag}(S_\ell) V_{\ell - 1}^{-1}
\]

where \( V_\ell \in \mathbb{R}^{n_\ell \times n_{\ell - 1}} \) are Haar distributed over orthonormal matrices and \( S_\ell = (s_{\ell,1}, \ldots, s_{\ell, \min(n_\ell, n_{\ell - 1})}) \). We will describe the distribution of the components \( S_\ell \) momentarily.

2) Assumption on Denoisers: We assume that the non-linear denoisers \( G^{\pm}_{2k} \) act row-wise on their inputs \( (R_{2k}, R_{2k - 1}) \). Further these operators and their Jacobian matrices \( \frac{\partial G^{\pm}_{2k}}{\partial R_{2k}}, \frac{\partial G^{\pm}_{2k}}{\partial R_{2k - 1}}, \frac{\partial G^{\pm}_{2k}}{\partial R_{2k - 1}} \) are uniformly Lipschitz continuous, the definition of which is provided in Appendix B.

3) Assumption on Initialization. True variables: The distribution of the remaining variables are described by a weak limit: For a matrix sequence \( X := X(N) \in \mathbb{R}^{d \times d} \), by the notation \( X \Rightarrow_x X \) we mean that there exists a random variable \( X \in \mathbb{R}^d \) with \( E \|X\|^2 < \infty \) such that \( \lim_{N \to \infty} \sum_{i=1}^{N} \psi(X_i) = E \psi(X) \) almost surely, for any bounded continuous function \( \psi : \mathbb{R}^d \to \mathbb{R} \), as well as for quadratic functions \( x^\top P x \) for any \( P \in \mathbb{R}^{d \times d} \). This is also referred to as Wasserstein-2 convergence [46]. For e.g., this property is satisfied for a random \( X \) with i.i.d. rows with bounded second moments, but is more general, since it applies to deterministic matrix sequences as well. More details on this weak limit are given in the Appendix B.

Let \( \overline{B}_\ell := \overline{V}_\ell^\top B_\ell \) and \( \overline{S}_\ell \in \mathbb{R}^{n_{\ell}^2} \) be the zero-padded vector of singular values of \( W_\ell \), and let \( \tau_{0\ell} \in \mathbb{R}^{2d \times d} \). Then we assume that the following empirical convergences hold,

\[
Z_0 \Rightarrow Z_0, \quad (\Xi_\ell, R_{0\ell} - Z_\ell^0) \Rightarrow (\Xi_\ell, Q_{0\ell}), \quad (S_\ell, B_\ell, \Xi_\ell, V_\ell^\top (R_{0\ell} - Z_0)) \Rightarrow (S_\ell, \overline{B}_\ell, \Xi_\ell, Q_{0\ell}), \quad \ell \text{ odd}
\]

where \( S_\ell \in \mathbb{R}^{2d \times d} \) is bounded, \( \overline{B}_\ell \in \mathbb{R}^{d \times d} \) is bounded, \( \Xi_\ell \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_{n_{\ell}^2}) \), and

\[
Q_{0\ell} \sim \mathcal{N}(\mathbf{0}, \tau_{0\ell}), \quad \ell = 0, 1, \ldots, L - 1
\]

are all pairwise independent random variables. We also assume that the sequence of initial matrices \( \{\Gamma_{0\ell}\} \) satisfy the following convergence pointwise

\[
\Gamma_{0\ell}(N) \to \Gamma_{0\ell}, \quad \ell = 0, 1, \ldots, L - 1
\]

B. Main Result

The main result of this paper concerns the empirical distribution of the rows \( Z_\ell^0[n], [R_\ell^0]_n \), of the iterates of Algorithm 1. It characterizes the asymptotic behaviour of these empirical distributions in terms of \( d \)-dimensional random vectors which are either Gaussians or functions of Gaussians. Let \( G^0_\ell \) denote maps \( \mathbb{R}^{1 \times d} \to \mathbb{R}^{1 \times d} \), such that (16), i.e.,

\[
|G^0_\ell (R_{0, -}, R_{0, +}, \Theta)|_n = G^0_\ell ([R_{0, -}]_n, [R_{0, +}]_n, \Theta).
\]

Having stated the requisite definitions and assumptions, we can now state our main result.

Theorem 1. For a fixed iteration index \( k \geq 0 \), there exist deterministic matrices \( K_{k\ell}^+ \in \mathbb{R}^{2d \times 2d} \), and \( \tau_{k\ell}, \Gamma_{k\ell}^+, \Gamma_{k\ell}^- \in \mathbb{R}^{d \times d} \) such that for even \( \ell \):

\[
\begin{pmatrix}
Z_{\ell - 1}^0 \\
Z_{\ell - 1}^+
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
G^0_\ell (C + \tilde{A}, B + A, \Gamma_{k\ell}^+, \Gamma_{k\ell}^-) \\
G^0_\ell (C + \tilde{A}, B + A, \Gamma_{k\ell}^+, \Gamma_{k\ell}^-)
\end{pmatrix}
\]

where \( (A, B) \sim \mathcal{N}(0, K_{k\ell}^+) \), \( C \sim \mathcal{N}(0, \tau_{k\ell}), \tilde{A} = \phi_\ell (A, \Xi_\ell) \) and \( (A, B) \), \( C \) are independent. For \( \ell = 0 \), the same result holds where the 1\textsuperscript{st} and 3\textsuperscript{rd} terms are dropped, whereas for \( \ell = L \), the 2\textsuperscript{nd} and 4\textsuperscript{th} terms are dropped.

Similarly, for odd \( \ell \):

\[
\begin{pmatrix}
V_{\ell - 1}^1 Z_{\ell - 1}^0 \\
V_{\ell - 1}^7 Z_{\ell - 1}^+
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
G^0_\ell (C + \tilde{A}, B + A, \Gamma_{k\ell}^+, \Gamma_{k\ell}^-) \\
G^0_\ell (C + \tilde{A}, B + A, \Gamma_{k\ell}^+, \Gamma_{k\ell}^-)
\end{pmatrix}
\]

where \( (A, B) \sim \mathcal{N}(0, K_{k\ell}^+) \), \( C \sim \mathcal{N}(0, \tau_{k\ell}), \tilde{A} = S_\ell A + \overline{B}_\ell + \Xi_\ell \) and \( (A, B) \), \( C \) are independent.

Furthermore for \( \ell = 0, 1, \ldots, L - 1 \), we have

\[
(G_{k\ell}^+, \Lambda_{k\ell}^+) \Rightarrow (T_{k\ell}^+, \Lambda_{k\ell}^+).
\]

The parameters in the distribution, \( \{K_{k\ell}^+, \tau_{k\ell}, \Gamma_{k\ell}^+, \Lambda_{k\ell}^+\} \) are deterministic and can be computed via a set of recursive equations called the "state evolution" or SE. The SE equations are provided in Appendix A. The result is similar to those for ML-VAMP in [17], [18] except that the SE equations for ML-Mat-VAMP involve \( d \times d \) and \( 2d \times 2d \) matrix terms; the ML-MAT-VAMP SE requires only require scalar and \( 2 \times 2 \) terms. The result holds for both MAP inference and MMSE inference, the only difference being implicit, i.e., the choice of denoiser \( G_\ell(\cdot) \) from eqn. (16).

The importance of Theorem 1 is that the rows of the iterates of the ML-Mat-VAMP Algorithm (\( Z_{k\ell}, a_{k\ell}, \hat{Z}_{k\ell} \) in Algorithm 1) and the rows of the corresponding true values, \( Z_{\ell - 1}^0, Z_{\ell}^0 \), have a simple, asymptotic random vector description of a typical row. We will call this the "row-wise" model. According to this model, for even \( \ell \), the rows of \( Z_{\ell - 1}^0 \) converge to a Gaussian \( \hat{Z}_{\ell}^0 \) and the rows of \( Z_{\ell}^0 \) converge to the output of the Gaussian through the row-wise function \( \phi_\ell, \hat{Z}_{\ell} = \phi_\ell (A, \Xi_\ell) \). Then the rows of the estimates \( Z_{\ell - 1}^- \), \( Z_{\ell}^+ \) asymptotically
We consider the problem of learning the input layer of a two layer neural network as described in Section II-C. We learn the weights $F_1$ of the first layer of a two-layer network by solving problem (12). The LSL analysis in this case corresponds to the input size $n_{in}$ and number of samples $N$ going to infinity with the number of hidden units being fixed. Our experiment take $d = 4$ hidden units, $N_{in} = 100$ input units, $N_{out} = 1$ output unit, sigmoid activations and variable number of samples $N$. The weight vectors $F_1$ and $F_2$ are generated as i.i.d. Gaussians with zero mean and unit variance. The input $X$ is also i.i.d. Gaussians with variance $1/N_{in}$ so that the average pre-activation has unit variance. Output noise is added at two levels of 10 and 15 dB relative to the mean. We generate 1000 test samples and a variable number of training samples that ranges from 200 to 4000. For each trial and number of training samples, we compare three methods: (i) MAP estimation where the MAP loss function is minimized by the ADAM optimizer [47] in the Keras package of Tensorflow; (ii) the M-VAMP algorithm run for 20 iterations and (iii) the M-VAMP state evolution prediction. The MAP-ADAM algorithm is run for 100 epochs with a learning rate = 0.01. The expectations in the M-VAMP SE are estimated via Monte-Carlo sampling (hence there is some variation).

Given an estimate $\hat{F}_1$ and true value $F_0$, we can compute the test error as follows: Given a new sample $x$, the true and predicted pre-activations will be $z_1 = (F_0^T)^T x$ and $\hat{z}_1 = \hat{F}_1^T x$. Thus, if the new sample $x \sim N(0, \frac{1}{N} I)$, the true and predicted pre-activations, $(z_1, \hat{z}_1)$, will be jointly Gaussian with covariance equal to the empirical $2d \times 2d$ covariance matrix of the rows of $F_0$ and $\hat{F}_1$:

$$K := \frac{1}{N_{in}} \sum_{k=1}^{N_{in}} u_k^F u_k^T, \quad u_k = \left[ F_{1,k}, \hat{F}_{1,k} \right]$$

From this covariance matrix, we can estimate the test error,

$$\mathbb{E}[|y - \hat{y}|^2] = \mathbb{E}[|F_0^T (\sigma(z_1) - \sigma(\hat{z}_1))|^2],$$

where the expectation is taken over the Gaussian $(z_1, \hat{z}_1)$ with covariance $K$. Also, since (26) is a row-wise operation, it can be predicted from the ML-Mat-V AMP SE. Thus, the SE can also predict the asymptotic test error. The normalized test error for ADAM-MAP, ML-Mat-V AMP and the ML-Mat-V AMP SE are plotted in Fig. 2. The normalized test error is defined as the ratio of the MSE on the test samples to the optimal MSE. Hence, a normalized MSE of one is the minimum value.

Note that since ADAM and ML-Mat-V AMP are solving the same optimization problem, they perform similarly as expected. The main message of this paper is not to develop an algorithm that outperforms ADAM, but rather an algorithm that has theoretical guarantees. The key property of ML-Mat-V AMP is that its asymptotic behavior at all the iterations can be exactly predicted by the state evolution equations. In this example, Fig. 2 shows that the normalized test MSE predicted via state evolution (plotted in green) matches the normalized MSE of ML-Mat-V AMP estimates (plotted in orange).

V. NUMERICAL EXPERIMENTS

We have developed a general framework for analyzing inference in multi-layer networks with matrix valued quantities in certain high-dimensional random settings. For learning the input layer of a two-layer network, the methods enables precise predictions of the expected test error as a function of the parameter statistics, numbers of samples and noise level. This analysis can thus in turn be valuable in understanding key properties such as generalization error. Future work will look to extend these to more complex networks.

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APPENDIX A. STATE EVOLUTION EQUATIONS

The state evolution equations given in Algo. 2 define an iteration indexed by $k$ of constant matrices $\{K_{kt}, \tau_k, \Gamma_k\}_{t=0}^L$. These constants appear in the statement of the main result in Theorem 1. The iterations in Algo. 2 also iteratively define a few $\mathbb{R}^{1\times d}$ valued random vectors $\{Q^t_0, P^t_0, Q^t_k, P^t_k\}$ which are either multivariate Gaussian or functions of Multivariate Gaussians. In order to state Algorithm 2, we need to define certain random variables and functions appearing therein which are described below. Let $L_{\text{odd}} = \{1, 3, \ldots, L-1\}$ and $L_{\text{even}} = \{2, 4, \ldots, L-2\}$.

Define $\{\Theta^\pm_{kt}\}$ similar to $\Theta^\pm_{kt}$ from equation (17) using $\{\Omega^\pm_{kt}\}$. Further, for $\ell = 1, 2, \ldots, L-1$ define
\[
\Omega^\pm_{kt} := (\Lambda_{kt}^+ \Gamma^+_{k,\ell} \Gamma_{k,\ell}^-), \quad \Omega^-_{kt} := (\Lambda_{k,\ell-1}^- \Gamma_{k,\ell-1}^- \Gamma_{k,\ell-1}^-),
\]
and $\Omega^-_{k0}$ and $\Omega_{kL}$. Now define random variables $W_\ell$ as
\[
W_0 = Z_0, \quad W_\ell = (Y, \Xi_\ell), \quad W_t = (S_t, \overline{B}_t, \Xi_t), \quad \forall \ell \in L_{\text{odd}},
\]
\[
W_\ell = (Y, \Xi_\ell), \quad \forall \ell \in L_{\text{even}} \cup \{L\},
\]
end for
(27)

Define functions $\{f^\pm_{kt}\}_{t=1}^L$ as
\[
f^0_{\ell} = \frac{\theta_{\ell}(P_{\ell-1}^+, W_t) \Gamma_{k,\ell}^- + \beta_{\ell}(t_0, Z_\ell)}{\Gamma_{k,\ell}^+}, \quad \forall \ell \in L_{\text{odd}},
\]
and using (17) define functions $\{h^\pm_{\ell}, \Gamma^\pm_{\ell}\}_{t=1}^L$, $h^0_{\ell}$ and $h^L_{\ell}$ as
\[
h^\pm_{\ell} = \frac{\theta_{\ell}(P_{\ell-1}^+, W_t, \Theta^\pm_{k,\ell})}{\Gamma^\pm_{k,\ell}}, \quad \forall \ell \in L_{\text{even}},
\]
\[
h^0_{\ell} = \frac{\theta_{\ell}(P_{\ell-1}^+, Q^t_0, W_t, \Theta^0_{k,\ell})}{\Gamma^0_{k,\ell}}, \quad \forall \ell \in L_{\text{odd}}
\]
end for
(29)

Note that $[G^+_{\ell}, G^-_{\ell}]$ and $[\tilde{G}^+_{\ell}, \tilde{G}^-_{\ell}]$ are maps from $\mathbb{R}^{1\times d} \rightarrow \mathbb{R}^{1\times d}$ such that their row-wise extensions are the denoisers $[G^+_{\ell}, G^-_{\ell}]$ and $[\tilde{G}^+_{\ell}, \tilde{G}^-_{\ell}]$ respectively. Using (29) define functions $\{f^\pm_{kt}\}_{t=1}^L$, $f^0_{\ell}$ and $f^L_{\ell}$ as
\[
f^\pm_{\ell} = \frac{\theta_{\ell}(P_{\ell-1}^+, P_{\ell-1}^+, W_t, \Omega^\pm_{k,\ell})}{\Gamma^0_{k,\ell}}, \quad \forall \ell \in L_{\text{even}}.
\]
\[
f^0_{\ell} = \frac{\theta_{\ell}(P_{\ell-1}^+, P_{\ell-1}^+, Q^t_0, W_t, \Omega^0_{k,\ell})}{\Gamma^0_{k,\ell}}, \quad \forall \ell \in L_{\text{odd}}
\]
end for
(30)

Algorithm 2: State Evolution for ML-Mat-VAMP (Algo. 1)

Require: Functions $\{f^0_{kt}\}$ from (28), $\{h^\pm_{kt}\}$ from (29), and $\{f^\pm_{kt}\}$ from (30). Perturbation random variables $\{W_\ell\}$ from (27). Initial random vectors $\{Q^t_0\}_{t=0}^{L-1}$ with Initial covariance matrices $\{\tau^t_k\}_{t=0}^{L-1}$ from (21). Initial matrices $\{\Omega^\pm_{k0}\}_{t=0}^{L-1}$ from (22).

1: // Initial Pass
2: $Q^t_0 = W_0$, $\tau^t_0 = \text{Cov}(Q^t_0)$ and $P^0_0 \sim \mathcal{N}(0, \tau^0_0)$
3: for $\ell = 1, \ldots, L-1$ do
4: $Q^t_\ell = f^0_{\ell}(P^0_{\ell-1}, W_\ell)$
5: $P^\ell_0 \sim \mathcal{N}(0, \tau^0_0)$, $\quad \Gamma^0_{k0} = \text{Cov}(Q^t_0, Q^t_{k0})$
6: end for

1: // Forward Pass
9: $Q^t_{k0} = h^0_{\ell}(Q^t_0, W_0, \Theta^0_{k0})$
10: $\overline{A}^+_{k0} = (\Sigma^t_{Q^t_0} \Sigma^{-1}_{Q^t_{k0}})^{-1} \Gamma^0_{k0}$
11: $\overline{A}^-_{k0} = \overline{A}^+_{k0} - \Gamma^0_{k0}$
12: $Q^t_{k} = f^+_{\ell}(P^0_{\ell-1}, P^+_{\ell-1}, Q^t_\ell, W_\ell, \overline{A}^+_{k0})$
13: $(P^0_{k0}, P^+_{k0}) \sim \mathcal{N}(0, \overline{K}^+_{k0})$, $\quad \overline{K}^+_{k0} := \text{Cov}(Q^0_0, Q^t_{k0})$

1: // Backward Pass
16: $\overline{A}^-_{kL} = (\Sigma^t_{Q^t_L} \Sigma^{-1}_{Q^t_{kL}})^{-1} \Gamma^0_{kL}$
17: $\overline{K}^+_{kL} = \overline{A}^-_{kL} - \Gamma^0_{kL}$
18: $Q^t_{kL} = f^-_{\ell}(P^0_{\ell-1}, P^-_{\ell-1}, Q^t_\ell, W_\ell, \overline{A}^-_{k0})$
19: $(P^0_{kL}, P^-_{kL}) \sim \mathcal{N}(0, \overline{K}^-_{kL})$, $\quad \overline{K}^-_{kL} := \text{Cov}(Q^0_0, Q^t_{kL})$

APPENDIX B. LARGE SYSTEM LIMIT DETAILS

The analysis of Algorithm 1 in the large system limit is based on [21] and is by now standard in the theory of AMP-based algorithms. The goal is to characterize ensemble row-wise averages of iterates of the algorithm using simpler finite-dimensional random variables which are either Gaussians or...
functions of Gaussians. To that end, we start by defining some key terms needed in this analysis.

**Definition 1** (Pseudo-Lipschitz continuity). For a given $p \geq 1$, a map $g : \mathbb{R}^{1 \times d} \to \mathbb{R}^{1 \times r}$ is called pseudo-Lipschitz of order $p$ if for any $r_1, r_2 \in \mathbb{R}^d$, we have,

$$\|g(r_1) - g(r_2)\| \leq C\|r_1 - r_2\| (1 + \|r_1\|^{p-1} + \|r_2\|^{p-1})$$

**Definition 2** (Empirical convergence of rows of a matrix sequence). Consider a matrix-sequence $\{X^{(N)}\}_{N=1}^{\infty}$ with $X^{(N)} \in \mathbb{R}^{N \times d}$. For a finite $p \geq 1$, let $X \in (\mathbb{R}^d, \mathcal{R}^d)$ be a $\mathcal{R}^d$-measurable random variable with bounded moment $\mathbb{E}\|X\|_p^\alpha < \infty$. We say the rows of matrix sequence $\{X^{(N)}\}$ converge empirically to $X$ with $p$th order moments if for all pseudo-Lipschitz continuous functions $f(\cdot)$ of order $p$,

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} f(X^{(N)}_n) = \mathbb{E}[f(X)] \quad \text{a.s.} \quad (31)$$

Note that the sequence $\{X^{(N)}\}$ could be random or deterministic. If it is random, however, then the quantities on the left hand side are random sums and the almost sure convergence must take this randomness into account as well.

The above convergence is equivalent to requiring weak convergence as well as convergence of the $p$th moment, of the empirical distribution $\frac{1}{N} \sum_{n=1}^{N} \delta_{X^{(N)}_n}$ of the rows of $X^{(N)}$ to $X$. This is also referred to convergence in the Wasserstein-$p$ metric [48, Chap. 6].

In the case of $p = 2$, the condition is equivalent to requiring (31) to hold for all continuously bounded functions $f$ as well as for all $f_q(x) = x^T Q x$ for all positive definite matrices $Q$.

**Definition 3** (Uniform Lipschitz continuity). For a positive definite matrix $M$, the map $\phi(r; M) : \mathbb{R}^d \to \mathbb{R}^d$ is said to be uniformly Lipschitz continuous in $r$ at $M = \overline{M}$ if there exist non-negative constants $L_1, L_2$ and $L_3$ such that for all $r \in \mathbb{R}^d$,

$$\|\phi(r_1; M_1) - \phi(r_2; M_2)\| \leq L_1\|r_1 - r_2\|$$

$$\|\phi(r; M_1) - \phi(r; M_2)\| \leq L_2(1 + \|r\|)\rho(M_1, M_2)$$

for all $M_i$ such that $\rho(M_i, \overline{M}) < L_3$, where $\rho$ is a metric on the cone of positive semidefinite matrices.

We are now ready to prove Theorem 1.

**APPENDIX C. PROOF OF THEOREM 1**

The proof of Theorem 1 is a special case of a more general result on multi-layer recursions given in Theorem 2. This result is stated in Appendix D, and proved in Appendix E. The rest of this section identifies certain relevant quantities from Theorem 1 in order to apply Theorem 2.

Consider the SVD given in equation (19) of weight matrices $W_\ell$ of the network. We analyze Algo. 1 using transformed versions of the true signals $Z^0_\ell$ and input errors $R^\pm_\ell - Z^0_\ell$ to the denoisers $G^\pm_\ell$. For $\ell = 0, 2, \ldots, L - 2$, define

$$q^0_\ell = Z^0_\ell \quad q^0_{\ell+1} = V^T_{\ell+1} Z^0_{\ell+1} \quad (32a)$$

$$p^0_\ell = V^T_\ell Z^0_\ell \quad p^0_{\ell+1} = Z^0_{\ell+1} \quad (32b)$$

which are depicted in Fig. 3 (TOP). Similarly, define the following transformed versions of errors in the inputs $R^\pm_\ell$ to the denoisers $G^\pm_\ell$

$$q^-_\ell = R^-_\ell - Z^0_\ell \quad q^-_{\ell+1} = V^T_{\ell+1} (R^-_{\ell+1} - Z^0_{\ell+1}) \quad (33a)$$

$$p^-_\ell = V_\ell (R^-_\ell - Z^0_\ell) \quad p^-_{\ell+1} = R^-_{\ell+1} - Z^0_{\ell+1} \quad (33b)$$

These quantities are depicted as inputs to function blocks $f^\pm_\ell$ in Fig. 3 (MIDDLE). Define perturbation variables $w_\ell$ as

$$w_0 = Z^0_0 \quad w_\ell = (Y_\ell, Z_\ell) \quad w_\ell = Z_\ell, \quad \forall \ell \in \mathcal{L}_{\text{even}} \quad (34a)$$

$$w_\ell = (S_\ell, B_\ell, \Xi_\ell), \quad \forall \ell \in \mathcal{L}_{\text{odd}} \quad (34b)$$

Finally, we define $q^+_\ell$ and $p^+_\ell$ for $\ell = 1, 2, \ldots, L - 1$ as

$$q^+_\ell = f^+_\ell (p^-_{\ell-1}, p^+_{\ell-1}, q^-_\ell, w_\ell, \Omega_\ell) \quad (35a)$$

$$p^+_\ell = f^+_\ell (p^-_{\ell-1}, p^+_{\ell-1}, q^-_\ell, w_\ell, \Omega_\ell) \quad (35b)$$

which are outputs of function blocks in Fig. 3 (MIDDLE). Similarly, define the quantities $q^0_\ell = f^0_\ell (q^0_0, Z^0_0, \Omega_0)$ and $p^0_{\ell+1} = f^0_\ell (p^0_\ell, p^0_{\ell+1}, Y_\ell, \Omega_\ell)$.

**Lemma 1.** Algorithm 1 is a special case of Algorithm 3 with the definitions $\{q^0_\ell, p^0_\ell, q^+_\ell, p^+_\ell\}_{\ell=0}^{L-1}$ given in equations (32), (33), and (35), functions $f^\pm_\ell$ are row-wise extensions of $f^0_\ell$ defined using equations (30) and (29).

**Lemma 2.** Assumptions 1 and 2 required for applying Theorem 2 are satisfied by the conditions in Theorem 1.

Proof. The proofs of the above lemmas are identical to the case of $d = 1$, which was shown in [18]. For details see [18, Appendix F].

**APPENDIX D. GENERAL MULTI-LAYER RECURSIONS**

To analyze Algorithm 1, we consider a more general class of recursions as given in Algorithm 3 and depicted in Fig. 3. The Gen-ML recursions generates (i) a set of true matrices $q^0_\ell$ and $p^0_\ell$ and (ii) iterated matrices $q^+_{\ell:}$ and $p^+_{\ell:}$. Each of these matrices have the same number of columns, denoted by $d$.

The true matrices are generated by a single forward pass, whereas the iterated matrices are generated via a sequence of forward and backward passes through a multi-layer system. In proving the State Evolution for the ML-Mat-VAMP algorithm (Algo. 1), one would then associate the terms $q^0_\ell$ and $p^0_\ell$ with certain error quantities in the ML-Mat-VAMP recursions. To account for the effect of the parameters $\Gamma^0_{\ell:k}$ and $\Delta^0_{\ell:k}$ in ML-Mat-VAMP, the Gen-ML algorithm describes the parameter updates through a sequence of parameter lists $\Gamma^0_{k:}$ and $\Delta^0_{k:}$. The parameter lists are ordered lists of parameters that accumulate as the algorithm progresses. The true and iterated matrices from Algorithm 3 are depicted in the signal flow graphs on the (TOP) and (MIDDLE) panel of Fig. 3 respectively. The iteration index $k$ for the iterated vectors $q_{k:}, p_{k:}$ has been dropped for simplifying notation.

The functions $f^0(\cdot)$ that produce the true matrices $q^0_\ell$, $p^0_\ell$ are called initial matrix functions and use the initial parameter list $\Theta^0_{0:}$. The functions $f^0_{\ell:k}(\cdot)$ that produce the matrices $q^0_{\ell:k}$ and $p^0_{\ell:k}$ are called the matrix update functions and use parameter
lists $\Upsilon_{kl}^\pm$. The initial parameter lists $\Upsilon_{01}$ are assumed to be provided. As the algorithm progresses, new parameters $\lambda_{kl}^\pm$ are computed and then added to the lists in lines 11, 17, 24 and 31. The matrix update functions $f_{kl}^\pm(\cdot)$ may depend on any sets of parameters accumulated in the parameter list. In lines 11, 17, 24 and 30, the new parameters $\lambda_{kl}^\pm$ are computed by: (1) computing average values $\mu_{kl}^\pm$ of row-wise functions $\phi_{kl}^\pm(\cdot)$; and (2) taking functions $\pi_{kl}^\pm(\cdot)$ of the average values $\mu_{kl}^\pm$. Since the average values $\mu_{kl}^\pm$ represent statistics on the rows of $\phi_{kl}^\pm(\cdot)$, we will call $\phi_{kl}^\pm(\cdot)$ the parameter statistic functions. We will call the $\pi_{kl}^\pm(\cdot)$ the parameter update functions. The functions $f_{kl}^\pm, f_{kl}^\pm, \phi_{kl}^\pm$ also take as input some perturbation vectors $w_k$.

Similar to the analysis of the ML-Mat-VAMP Algorithm, we consider the following large-system limit (LSL) analysis of Gen-ML. Specifically, we consider a sequence of runs of the recursions indexed by $N$. For each $N$, let $N_\ell = N_\ell(N)$ be the dimension of the matrix signals $p_k^\pm$ and $q_k^\pm$ as we assume $0 < \beta_\ell \leq 1$. Note however that the number of columns of each of the matrices $\{q_k^0, p_k^0, q_k^+, p_k^+(\cdot), q_k^-, p_k^-(\cdot)\}$ is equal to a finite integer $d > 0$, which remains fixed for all $N$. We then make the following assumptions. See Appendix B for an overview of empirical convergence of sequences which we use in the assumptions described below.

**Assumption 1.** For vectors in the Gen-ML Algorithm (Algorithm 3), we assume:

(a) The matrices $V_k$ are Haar distributed on the set of $N_\ell \times N_\ell$ orthogonal matrices and are independent from one another and from the matrices $q_k^0, q_k^\pm$, perturbation variables $w_k$.

(b) The rows of the initial matrices $q_k^0$, and perturbation variables $w_k$ converge jointly empirically with limits,

$$q_k \overset{2}{\Rightarrow} Q_{0k}, \quad w_k \overset{2}{\Rightarrow} W_k,$$

where $Q_{0k}$ are random vectors in $\mathbb{R}^{1 \times d}$ such that $(Q_{0k,0}, \ldots, Q_{0k,L-1})$ is jointly Gaussian. For $k = 0, \ldots, L-1$, the random variables $W_k, P_k$ and $Q_{0k}$ are all independent. We also assume that the initial parameter list converges as

$$\lim_{N \to \infty} \Upsilon_{01}(N) \overset{a.s.}{\Rightarrow} \Upsilon_{01},$$

for some list $\Upsilon_{01}$. The limit (37) means that every element in the list $\lambda(N) \in \Upsilon_{01}(N)$ converges to a limit $\lambda(N) \in \Upsilon_{01}$ as $N \to \infty$ almost surely.

(c) The matrix update functions $f_{kl}^\pm(\cdot)$ and parameter update functions $\phi_{kl}^\pm(\cdot)$ act row-wise. For e.g., in the $k^{th}$ forward pass, at stage $\ell$, we assume that for each output row $n$,

$$f_{kl}^\pm(p_{k-1,0}; p_{k-1,0}^+, q_{k}, w_{k}, \Upsilon_{kl}^\pm)[n] :\begin{cases}
\sum_{\ell \neq k} \alpha_{nk}^{k \ell} f_{k\ell}^+(p_{k-1,0}^+, p_{k-1,0}^+, q_{k}, w_{k}, \Upsilon_{k\ell}^\pm)[n] \\
\sum_{\ell \neq k} \alpha_{nk}^{k \ell} f_{k\ell}^-(p_{k-1,0}^-, p_{k-1,0}^-, q_{k}, w_{k}, \Upsilon_{k\ell}^\pm)[n] \\
\sum_{\ell \neq k} \alpha_{nk}^{k \ell} f_{k\ell}^\pm(p_{k-1,0}^\pm, p_{k-1,0}^\pm, q_{k}, w_{k}, \Upsilon_{k\ell}^\pm)[n]
\end{cases}$$

Fig. 3. (TOP) The equations (1) with equivalent quantities defined in (32), and $f_k^0$ defined using (28).

(MIDDLE) The Gen-ML-Mat recursions in Algorithm 3. These are also equivalent to ML-Mat-VAMP recursions from Algorithm 1 (See Lemma 1) if $q_k^\pm, p_k^\pm$ are as defined in equations (33) and (35), and $f_k^\pm$ given by equations (30) and (29).

(BOTTOM) Quantities in the GEN-ML-SE recursions. These are also equivalent to ML-Mat-VAMP SE recursions from Algorithm 2 (See Lemma 1). The iterations $k$ have been dropped for notational simplicity.
Algorithm 3 General Multi-Layer Matrix (Gen-ML-Mat) Recursion

Require: Initial matrix functions \( \{f^0_p\} \). Matrix update functions \( \{f^\lambda_p(\cdot)\} \). Parameter statistic functions \( \{\varphi^\lambda_p(\cdot)\} \). Parameter update functions \( \{T^\lambda_{kl}\} \). Orthogonal matrices \( \{V_\ell\} \). Perturbation variables \( \{w^\ell_p\} \). Initial matrices \( \{q^0_{kl}\} \).

Initial parameter list \( Y_{01} \).

1: // Initial Pass
2: \( q^0_{kl} = f^0_p(w_0) \), \( p^0_{kl} = V_{0} q^0_{kl} \)
3: for \( \ell = 1, \ldots, L-1 \) do
4: \( q^\ell_{kl} = f^\ell_p(p^\ell_{k-1,l}, w_\ell, Y_{01}) \)
5: \( p^\ell_{kl} = V_{\ell} q^\ell_{kl} \)
6: end for
7: for \( k = 0, 1, \ldots \) do
8: // Forward Pass
9: \( \lambda^\ell_{k0} = T^{\ell}_{k0}(\mu^0_{k0}, Y_{0k}) \)
10: \( \mu^\ell_{k0} = \langle \varphi^\ell_{k0}(q^\ell_{k0}, w_0, Y_{0k}) \rangle \)
11: \( Y^\ell_{k0} = \langle Y_{k0}^{\ell-1}, \lambda^\ell_{k0} \rangle \)
12: \( q^\ell_{k0} = f^\ell_p(q^\ell_{k0}, w_0, Y^\ell_{k0}) \)
13: \( p^\ell_{k0} = V_{0} q^\ell_{k0} \)
14: \( \lambda^\ell_{kl} = T^{\ell}_{kl}(\mu^\ell_{k0}, Y^\ell_{kl-1}) \)
15: \( \mu^\ell_{kl} = \langle \varphi^\ell_{kl}(p^\ell_{k-1,l}, w_L, Y^\ell_{kl-1}) \rangle \)
16: \( Y^\ell_{kl} = \langle Y^\ell_{k-1,l}, \lambda^\ell_{kl} \rangle \)
17: \( q^\ell_{kl} = f^\ell_p(p^\ell_{k-1,l}, w_L, Y^\ell_{kl}) \)
18: \( p^\ell_{kl} = V_{\ell} q^\ell_{kl} \)
19: end for
20: // Backward Pass
21: \( \lambda^{k1,L} = T^{-1}_{k1,L}(\mu^{k1,L}, Y^{-1}_{k1,L}) \)
22: \( \mu^{k1,L} = \langle \varphi^{k1,L}(p^{k1,L}, w_L, Y^{-1}_{k1,L}) \rangle \)
23: \( Y^{k1,L} = \langle Y^{k1-1,L}, \lambda^{k1,L} \rangle \)
24: \( q^{k1,L} = f^{k1,L}(p^{k1,L}, w_L, Y^{k1,L}) \)
25: \( p^{k1,L} = V_{L} q^{k1,L} \)
26: for \( \ell = L-1, \ldots, 1 \) do
27: \( \lambda^{k1,\ell} = T^{-1}_{k1,\ell}(\mu^{k1,\ell}, Y^{-1}_{k1,\ell}) \)
28: \( \mu^{k1,\ell} = \langle \varphi^{k1,\ell}(p^{k1,\ell}, w_L, Y^{-1}_{k1,\ell}) \rangle \)
29: \( Y^{k1,\ell} = \langle Y^{k1-1,\ell}, \lambda^{k1,\ell} \rangle \)
30: \( q^{k1,\ell} = f^{k1,\ell}(p^{k1,\ell}, w_L, Y^{k1,\ell}) \)
31: \( p^{k1,\ell} = V_{\ell} q^{k1,\ell} \)
32: end for
33: end for
34: end for
35: end for

\[
\left[ \varphi^\ell_{kl}(p^\ell_{k-1,l}, p^\ell_{k-1,l}, q^\ell_{kl}, w_\ell, Y^\ell_{kl}) \right]_n = \varphi^\ell_{kl}(p^\ell_{k-1,l}, q^\ell_{kl}, w_\ell, Y^\ell_{kl})
\]

for some \( R^{k \times d} \)-valued functions \( f^\ell_{kl}(\cdot) \) and \( \varphi^\ell_{kl}(\cdot) \). Similar definitions apply in the reverse directions and for the initial vector functions \( f^0_p(\cdot) \). We will call \( f^\ell_{kl}(\cdot) \) the matrix update row-wise functions and \( \varphi^\ell_{kl}(\cdot) \) the parameter update row-wise functions.

Next we define a set of deterministic constants \( \{K^\ell_{kl}, T^\ell_{kl}, P^\ell_{kl}, \varphi^\ell_{kl}, \lambda^\ell_{kl}, \mu^\ell_{kl} \} \) and \( R^{k \times d} \)-valued random vectors \( \{Q^0_p, P^0_{kl}, Q^0_{kl}, P^0_{kl} \} \) which are recursively defined through Algorithm 4, which we call the Gen-ML-Mat State Evolution (SE). These recursions in Algorithm closely mirror those in

Algorithm 4 Gen-ML-Mat State Evolution (SE)

Require: Matrix update row-wise functions \( f^\ell_p(\cdot) \) and \( f^{k1,L}_p(\cdot) \), parameter statistic row-wise functions \( \varphi^\ell_p(\cdot) \), parameter update functions \( T^\ell_{kl}(\cdot) \), initial parameter list limit: \( Y_{01} \), initial random variables \( W_\ell, Q^0_{kl}, \ell = 0, \ldots, L-1 \).

1: // Initial pass
2: \( Q^0_p = f^0_p(W_0, Y_{01}) \), \( P^0_{kl} \sim \mathcal{N}(0, \tau^0_0) \), \( \tau^0_0 = \mathbb{E}(Q^0_p)^2 \)
3: for \( \ell = 1, \ldots, L-1 \) do
4: \( Q^\ell_p = f^\ell_p(P^0_{\ell-1}, W_\ell, Y_{01}) \)
5: \( P^\ell_p \sim \mathcal{N}(0, \tau^\ell_p) \), \( \tau^\ell_p = \mathbb{E}(Q^\ell_p)^2 \)
6: end for
7: for \( k = 0, 1, \ldots \) do
8: // Forward Pass
9: \( Y^\ell_{k0} = T^\ell_{k0}(\mu^0_{k0}, Y_{0k}) \)
10: \( \mu^\ell_{k0} = \mathbb{E}(\varphi^\ell_{k0}(Q^\ell_0, W_0, Y_{0k})) \)
11: \( Y^\ell_{k0} = \mathbb{E}(\varphi^\ell_{k0}(Q^\ell_0, W_0, Y^\ell_{k0})) \)
12: \( Q^\ell_{k0} = f^\ell_p(Q^\ell_0, W_0, Y^\ell_{k0}) \)
13: \( (P^0_{k0}, P^0_{k0}) \sim \mathcal{N}(0, \mathbf{K}_0) \), \( \mathbf{K}^\ell_{k0} = \mathbb{E}(Q^\ell_p, Q^\ell_{kl}) \)
14: for \( \ell = 1, \ldots, L-1 \) do
15: \( Y^\ell_{kl} = T^\ell_{kl}(\mu^\ell_{k0}, Y^\ell_{kl-1}) \)
16: \( Q^\ell_{kl} = f^\ell_p(P^0_{k-1,l}, P^0_{k-1,l}, Q^\ell_{k-1,l}, W_\ell, Y^\ell_{k-1,l}) \)
17: \( \mathbf{K}^\ell_{kl} = \mathbb{E}(Q^\ell_p, Q^\ell_{kl}) \)
18: \( \lambda^{k1,L} = T^{-1}_{k1,L}(\mu^{k1,L}, Y^{-1}_{k1,L}) \)
19: \( \mu^{k1,L} = \mathbb{E}(\varphi^{k1,L}(P^0_{k1,L}, W_L, Y^{-1}_{k1,L})) \)
20: \( \mathbf{K}^\ell_{k1,L} = \mathbb{E}(P^0_{k1,L}, P^0_{k1,L}, W_L, Y^{-1}_{k1,L}) \)
21: \( Q^\ell_{k1,L} \sim \mathcal{N}(0, \mathbf{K}^\ell_{k1,L}) \), \( \mathbf{K}^\ell_{k1,L} = \mathbb{E}(Q^\ell_p, Q^\ell_{k1,L}) \)
22: end for
23: \( K^\ell_{k1,L} = T^\ell_{k1,L}(\mu^\ell_{k0}, Y^\ell_{k1,L}) \)
24: \( P^\ell_{k1,L} = f^\ell_p(P^0_{k1,L}, P^0_{k1,L}, Q^\ell_{k1,L}, W_L, Y^\ell_{k1,L}) \)
25: \( Q^\ell_{k1,L} \sim \mathcal{N}(0, \tau^\ell_{k1,L}) \), \( \tau^\ell_{k1,L} = \mathbb{E}(Q^\ell_p, Q^\ell_{k1,L}) \)
26: for \( \ell = L-1, \ldots, 1 \) do
27: \( Y^\ell_{k1,L} = T^{-1}_{k1,L}(\mu^\ell_{k0}, Y^{-1}_{k1,L}) \)
28: \( P^\ell_{k1,L} = f^\ell_p(P^0_{k1,L}, P^0_{k1,L}, Q^\ell_{k1,L}, W_L, Y^{-1}_{k1,L}) \)
29: \( Q^\ell_{k1,L} \sim \mathcal{N}(0, \tau^\ell_{k1,L}) \), \( \tau^\ell_{k1,L} = \mathbb{E}(Q^\ell_p, Q^\ell_{k1,L}) \)
30: end for
31: end for
the Gen-ML-Mat algorithm (Algorithm 3). The matrices \( \mathbf{q}_{i,k}^+ \) and \( \mathbf{p}_{k}^+ \) are replaced by random vectors \( Q_{i,k}^+ \) and \( P_{k}^+ \); the matrix and parameter update functions \( f_{k}(\cdot) \) and \( \varphi_{k}(\cdot) \) are replaced by their row-wise functions \( f_{k}^{+}(\cdot) \) and \( \varphi_{k}^{+}(\cdot) \); and the parameters \( \lambda_{k}^+ \) are replaced by their limits \( \lambda_{k}^+ \). We refer to \( \{Q_{i,k}^+, P_{k}^+\} \) as true random vectors and \( \{Q_{i,k}^+, P_{k}^+\} \) as iterated random vectors. The signal flow graph for the true and iterated random variables in Algorithm 4 is given in the (BOTTOM) panel of Fig. 3. The iteration index \( k \) for the iterated random variables \( \{Q_{i,k}^+, P_{k}^+\} \) to simplify notation.

We also assume the following about the behaviour of row-wise functions around the quantities defined in Algorithm 4. The iteration index \( k \) has been dropped for simplifying notation.

**Assumption 2.** For row-wise functions \( f, \varphi \) and parameter update functions \( T \) we assume:

(a) \( T_{k}^{\pm}(\mu_{k}^{\pm}, \cdot) \) are continuous at \( \mu_{k}^{\pm} = \mathbf{m}_{k}^{\pm} \)

(b) \( f_{k}^{+}(p_{k}^{+}, q_{k}^{+}, \ldots, P_{k}^{+}, Q_{k}^{+}, w_{k}, Y_{k}^{+}) \) and \( \varphi_{k}^{+}(p_{k}^{+}, q_{k}^{+}, \ldots, P_{k}^{+}, Q_{k}^{+}, w_{k}, Y_{k}^{+}) \) are uniformly Lipschitz continuous in \( (p_{k}^{+}, q_{k}^{+}, \ldots, P_{k}^{+}, Q_{k}^{+}, w_{k}) \) at \( Y_{k}^{+} = Y_{k}^{+} \)

(c) \( f_{k}^{0}(p_{k}^{0}, w_{k}) = Y_{0}^{+} \) uniformly Lipschitz continuous in \( (p_{k}^{0}, w_{k}) \) at \( Y_{k=1}^{+} = Y_{k=1}^{+} \)

(d) Matrix update functions \( f_{k}^{+}(\cdot) \) are asymptotically divergence free meaning

\[
\lim_{N \to \infty} \left\langle \frac{\partial f_{k}(\cdot)}{\partial p_{k}^{+}}(p_{k}^{+}, q_{k}^{+}, \ldots, P_{k}^{+}, Q_{k}^{+}, w_{k}, Y_{k}^{+}) \rightangle = 0,
\]

\[
\lim_{N \to \infty} \left\langle \frac{\partial \varphi_{k}(\cdot)}{\partial p_{k}^{+}}(p_{k}^{+}, q_{k}^{+}, \ldots, P_{k}^{+}, Q_{k}^{+}, w_{k}, Y_{k}^{+}) \rightangle = 0.
\]

We are now ready to state the general result regarding the empirical convergence of the true and iterated vectors from Algorithm 3 in terms of random variables defined in Algorithm 4.

**Theorem 2.** Consider the iterates of the Gen-ML recursion (Algorithm 3) and the corresponding random variables and parameter limits defined by the SE recursions (Algorithm 4) under Assumptions 1 and 2. Then,

(a) For any fixed \( k \geq 0 \) and fixed \( \ell = 1, \ldots, L - 1 \), the parameter list \( Y_{k \ell}^{+} \) converges as

\[
\lim_{N \to \infty} Y_{k \ell}^{+} = Y_{k \ell}^{+}
\]

almost surely. Also, the rows of \( \mathbf{m}_{k}^{0}, \mathbf{q}_{0}^{0}, \mathbf{p}_{0,k}^{+}, \ldots, \mathbf{p}_{k}^{+}, \mathbf{q}_{k}^{+} \) and \( \mathbf{q}_{0}^{0}, \mathbf{p}_{0,k}^{+}, \ldots, \mathbf{p}_{k}^{+} \) almost surely jointly converge empirically with limits,

\[
(\mathbf{p}_{k \ell}^{0}, \mathbf{p}_{k \ell}^{+}, \mathbf{q}_{j \ell}, \mathbf{q}_{j \ell}^{0}, \mathbf{q}_{j \ell}^{+}) \to (\mathbf{p}_{k \ell}^{0}, \mathbf{p}_{k \ell}^{+}, \mathbf{Q}_{j \ell}^{0}, \mathbf{Q}_{j \ell}^{+}),
\]

for all \( 0 \leq i, j \leq k \), where the variables \( \mathbf{p}_{k \ell}^{0}, \mathbf{p}_{k \ell}^{+} \) and \( \mathbf{Q}_{j \ell}^{0}, \mathbf{Q}_{j \ell}^{+} \) are zero-mean jointly Gaussian random variables independent of \( \mathbf{W}_{\ell} \) and with covariance matrix given by

\[
\text{Cov}(\mathbf{p}_{k \ell}^{0}, \mathbf{p}_{k \ell}^{+}) = \mathbf{K}_{k \ell}^{+}, \quad \mathbb{E}(\mathbf{Q}_{j \ell}^{0}) = \mathbf{K}_{j \ell}^{+},
\]

\[
\mathbb{E}(\mathbf{p}_{k \ell}^{+}^T \mathbf{Q}_{j \ell}^{+}) = 0, \quad \mathbb{E}(\mathbf{p}_{k \ell}^{+}) = 0,
\]

and \( \mathbf{Q}_{j \ell}^{0}, \mathbf{Q}_{j \ell}^{+} \) are the random variable in lines 4, 19, i.e.,

\[
\mathbf{Q}_{j \ell}^{0} = f_{j \ell}^{0}(\mathbf{p}_{0,1}, \mathbf{W}_{\ell}), \quad \mathbf{Q}_{j \ell}^{+} = f_{j \ell}^{+}(\mathbf{p}_{0,1}, \mathbf{p}_{k \ell}^{+}, \mathbf{Q}_{j \ell}^{0}, \mathbf{W}_{\ell}, \mathbf{Y}_{k \ell}^{+}).
\]

An identical result holds for \( \ell = 0 \) with all the variables \( \mathbf{p}_{k}^{0}, \mathbf{p}_{k}^{+} \) removed.

(b) For any fixed \( k \geq 1 \) and fixed \( \ell = 1, \ldots, L - 1 \), the parameter lists \( Y_{k \ell}^{0} \) converge as

\[
\lim_{N \to \infty} Y_{k \ell}^{0} = Y_{k \ell}^{0}
\]

almost surely. Also, the rows of \( \mathbf{w}_{\ell}, \mathbf{p}_{0,1}^{0}, \mathbf{p}_{0,k}^{0}, \ldots, \mathbf{p}_{k}^{0}, \mathbf{q}_{0}^{0}, \ldots, \mathbf{q}_{k}^{0} \) almost surely jointly converge empirically with limits,

\[
(\mathbf{p}_{k \ell}^{0}, \mathbf{p}_{k \ell}^{+}, \mathbf{q}_{j \ell}, \mathbf{q}_{j \ell}^{0}, \mathbf{q}_{j \ell}^{+}) \to (\mathbf{p}_{k \ell}^{0}, \mathbf{p}_{k \ell}^{+}, \mathbf{Q}_{j \ell}^{0}, \mathbf{Q}_{j \ell}^{+}),
\]

for all \( 0 \leq i, j \leq k \), where the variables \( \mathbf{p}_{k \ell}^{0}, \mathbf{p}_{k \ell}^{+} \) and \( \mathbf{Q}_{j \ell}^{0}, \mathbf{Q}_{j \ell}^{+} \) are zero-mean jointly Gaussian random variables independent of \( \mathbf{W}_{\ell} \) and with covariance matrix given by equation (41) and \( \mathbf{p}_{k \ell}^{+} \) is the random variable in line 32:

\[
\mathbf{p}_{k \ell}^{+} = f_{j \ell}^{0}(\mathbf{p}_{0,1}, \mathbf{p}_{k \ell}^{0}, \mathbf{Q}_{j \ell}^{0}, \mathbf{W}_{\ell}, \mathbf{Y}_{k \ell}^{0}).
\]

An identical result holds for \( \ell = L \) with all the variables \( \mathbf{q}_{j \ell}^{0} \) and \( \mathbf{Q}_{j \ell}^{0} \) removed.

For \( k = 0 \), \( Y_{0 \ell}^{0} \to Y_{0 \ell}^{0} \) almost surely, and the rows \( \{(\mathbf{w}_{\ell,n}, \mathbf{p}_{k \ell}^{0}, \mathbf{q}_{j \ell}^{0}, \mathbf{q}_{j \ell}^{+})\}_{n=1}^{N} \) empirically converge to independent random variables \( \{(\mathbf{w}_{\ell}, \mathbf{p}_{k \ell}^{0}, \mathbf{q}_{j \ell}^{0})\}_{n=1}^{N} \).

**Proof.** Appendix E is dedicated to proving this result. □

**APPENDIX E. PROOF OF THEOREM 2**

The proof proceeds using mathematical induction. It largely mimics the proof for the case of \( d = 1 \) which were the convergence results in [18, Thm. 5]. However, in the case of \( d > 1 \), we observe that several quantities which were scalars in proving [18, Thm. 5] are now matrices. Due to the noncommutativity of these matrix quantities, we re-state the whole prove, while modifying the requisite matrix terms appropriately.

**A. Overview of the Induction Sequence**

The proof is similar to that of [26, Theorem 4], which provides a SE analysis for VAMP on a single-layer network. The critical challenge here is to extend that proof to multi-layer
recursions. Many of the ideas in the two proofs are similar, so we highlight only the key differences between the two.

Similar to the SE analysis of VAMP in [26], we use an induction argument. However, for the multi-layer proof, we must index over both the iteration index $k$ and layer index $\ell$. To this end, let $H_{k\ell}^+$ and $H_{k\ell}^-$ be the hypotheses:

- $H_{k\ell}^+$: The hypothesis that Theorem 2(a) is true for a given $k$ and $\ell$, with $0 \leq \ell \leq L - 1$.
- $H_{k\ell}^-$: The hypothesis that Theorem 2(b) is true for a given $k$ and $\ell$, with $1 \leq \ell \leq L$.

We prove these hypotheses by induction via a sequence of implications,

$$\{H_{0\ell}^+\}_{\ell=1}^L \Rightarrow H_{k1}^+ \Rightarrow \cdots \Rightarrow H_{L1}^+ \Rightarrow \cdots \Rightarrow H_{k1}^- \Rightarrow \cdots \Rightarrow H_{kL}^- \Rightarrow \cdots,$$

beginning with the hypotheses $\{H_{0\ell}^\pm\}$ for all $\ell = 1, \ldots, L-1$.

**B. Case Base: Proof of $H_{0\ell}^+$**

The base case corresponds to the hypotheses $\{H_{0\ell}^+\}_{\ell=1}^L$. Note that Theorem 2(b) states that for $k = 0$, we need $T_{01} \rightarrow T_{01}$ almost surely, and $\{(w_{\ell,n}, p_{01}^0, q_{0\ell,n}^-)\}_{n=1}^\infty$ empirically converge to independent random variables $(W_{\ell}, P_{01}^0, Q_{0\ell}^-)$. These follow directly from equations (36) and (37) in Assumption 1 (a).

**C. Inductive Step: Proof of $H_{k\ell+1}^+$**

Fix a layer index $\ell = 1, \ldots, L-1$ and an iteration index $k = 1, \ldots, L-1$. We show the implication $\cdots \Rightarrow H_{k\ell+1}^+ \Rightarrow \cdots$, which can be proven similarly using symmetry arguments.

**Definition 4** (Induction hypothesis). The hypotheses prior to $H_{k\ell+1}^+$ in the sequence (46), but not including $H_{k\ell+1}^+$, are true.

The inductive step then corresponds to the following result.

**Lemma 3. Under the induction hypothesis, $H_{k\ell+1}^+$ holds**

Before proving the inductive step in Lemma 3, we prove two intermediate lemmas. Let us start by defining some notation. Define $P_{k\ell}^\pm := \{ p_{k\ell,\ell}^+ \}_{\ell=1}^L \in \mathbb{R}^{N_k \times (k+1)d}$, be a matrix whose column blocks are the first $k+1$ values of the matrix $p_{k\ell}^\pm$. We define the matrices $P_{k\ell}^\pm$, $Q_{k\ell}^\pm$ and $Q_{k\ell}^0$ in a similar manner with values of $p_{k\ell}^\pm$, $q_{k\ell}^\pm$ and $q_{k\ell}^0$, respectively.

Note that except the initial matrices $\{w_{\ell}, q_{0\ell}^0\}_{\ell=1}^L$, all later iterates in Algorithm 3 are random due to the randomness of $V_{\ell}$. Let $\mathcal{G}_{k\ell}^\pm$ denote the collection of random variables associated with the hypotheses, $H_{k\ell}^\pm$. That is, for $\ell = 1, \ldots, L$,

$$\mathcal{G}_{k\ell}^+ := \{w_{\ell}, p_{k\ell,\ell}^+, Q_{k\ell}^+, Q_{k\ell}^+, Q_{k\ell}^+, Q_{k\ell}^+\},$$

$$\mathcal{G}_{k\ell}^- := \{w_{\ell}, p_{k\ell,\ell}^-, Q_{k\ell}^-, Q_{k\ell}^-, Q_{k\ell}^-, Q_{k\ell}^+\}.$$

For $\ell = 0$ and $\ell = L$ we set, $\mathcal{G}_{k0}^+ := \{w_{0}, Q_{k0}^+, Q_{k0}^+\}$, $\mathcal{G}_{kL}^+ := \{w_{\ell}, P_{k\ell-1}^0, P_{k\ell-1}^+, P_{k\ell-1}^-, P_{k\ell-1}^-\}$.

Let $\mathcal{F}_{k\ell}^\pm$ be the sigma algebra generated by the union of all the sets $\mathcal{G}_{k\ell}^\pm$ as they have appeared in the sequence (46) up to and including the final set $\mathcal{G}_{kL}^\pm$. Thus, the sigma algebra $\mathcal{F}_{k\ell}^\pm$ contains all information produced by Algorithm 3 immediately before line 20 in layer $\ell$ of iteration $k$. Note also that the random variables in Algorithm 4 immediately before defining $P_{k\ell}^\pm$ in line 20 are all $\mathcal{F}_{k\ell}^\pm$ measurable.

Observe that the matrix $V_{\ell}$ in Algorithm 3 appears only during matrix-vector multiplications in lines 20 and 32. If we define the matrices, $A_{k\ell} := [p_{k\ell,\ell}^+, P_{k\ell-1}^+, P_{k\ell}^+, P_{k\ell}^-]$ and $B_{k\ell} := [q_{k\ell}^+, Q_{k\ell}^-, Q_{k\ell}^+, Q_{k\ell}^+]$, all the matrices in the set $\mathcal{G}_{k\ell}$ will be unchanged for all matrices $V_{\ell}$ satisfying the linear constraints

$$\mathbf{A}_{k\ell} = V_{\ell} \mathbf{B}_{k\ell}.$$

Hence, the conditional distribution of $V_{\ell}$ given $\mathcal{F}_{k\ell}$ is precisely the uniform distribution on the set of orthogonal matrices satisfying (47). The matrices $A_{k\ell}$ and $B_{k\ell}$ are of dimensions $N_{\ell} \times (2k+2)d$. From [26, Lemmas 3.4], this conditional distribution is given by

$$V_{\ell} \mid \mathcal{F}_{k\ell} \overset{d}{=} A_{k\ell}(A_{k\ell}^T A_{k\ell})^{-1} B_{k\ell}^T + U_{A_{k\ell}} \mathbf{V}_{\ell} U_{A_{k\ell}}^T,$$

where $U_{A_{k\ell}}$ and $U_{B_{k\ell}}$ are $N_{\ell} \times (N_{\ell} - (2k+2)d)$ matrices whose columns are an orthonormal basis for $\text{Range}(A_{k\ell})^\perp$ and $\text{Range}(B_{k\ell})^\perp$. The matrix $\mathbf{V}_{\ell}$ is Haar distributed on the set of $(N_{\ell} - (2k+2)d) \times (N_{\ell} - (2k+2)d)$ orthogonal matrices and is independent of $\mathcal{F}_{k\ell}$.

Next, similar to the proof of [26, Thm. 4], we can use (48) to write the conditional distribution of $p_{k\ell}^\pm$ (from line 20 of Algorithm 3) given $\mathcal{F}_{k\ell}$ as a sum of two terms

$$p_{k\ell}^\pm \mid \mathcal{F}_{k\ell} = V_{\ell} \mid \mathcal{F}_{k\ell} q_{k\ell}^\pm = P_{k\ell}^\pm + p_{k\ell}^\text{ran},$$

$$p_{k\ell}^\text{ran} := U_{B_{k\ell}}^T V_{\ell} U_{A_{k\ell}}^T q_{k\ell}^\pm,$$

where we call $p_{k\ell}^\text{det}$ the deterministic term and $p_{k\ell}^\text{ran}$ the random term. The next two lemmas characterize the limiting distributions of the deterministic and random terms.

**Lemma 4. Under the induction hypothesis, the rows of the “deterministic” term $P_{k\ell}^\text{det}$ along with the rows of the matrices in $\mathcal{G}_{k\ell}^\pm$ converge empirically. In addition, there exists constant $d \times d$ matrices $\beta^\text{det}_0, \ldots, \beta^\text{det}_{k-1, \ell}$ such that

$$p_{k\ell}^\text{det} \overset{d}{\Rightarrow} p_{k\ell}^\text{det} := P_{k\ell}^\text{det} + \sum_{i=0}^{k-1} P_{i\ell}^\text{det} \beta_{i\ell},$$

where $p_{k\ell}^\text{det} \in \mathbb{R}^{1 \times d}$ is the limiting random vector for the rows of $p_{k\ell}^\text{det}$.

**Proof.** The proof is similar to that of [26, Lem. 6], but we go over the details as there are some important differences in the multi-layer case. Define $\tilde{P}_{k\ell} := [p_{k\ell,\ell}, P_{k\ell}^+, P_{k\ell}^-]$ and $\tilde{Q}_{k\ell} := [q_{k\ell,\ell}, Q_{k\ell}^+, Q_{k\ell}^-]$, which are the matrices in $\mathbb{R}^{N_{\ell} \times (k+1)d}$. We can
then write $A_{k\ell}$ and $B_{k\ell}$ from (47) as

$$A_{k\ell} := \left[ \bar{P}_{k-1,\ell}^+ P_{k\ell}^- \right], \quad B_{k\ell} := \left[ \bar{Q}_{k-1,\ell}^+ \bar{Q}_{k\ell}^- \right], \quad (51)$$

We first evaluate the asymptotic values of various terms in (49b). By definition of $B_{k\ell}$ in (51),

$$B_{k\ell}^T B_{k\ell} = \left[ \left( \bar{Q}_{k-1,\ell}^+ \right)^T \bar{Q}_{k-1,\ell}^- \right] \left( \bar{Q}_{k\ell}^- \right)^T \bar{Q}_{k\ell}^+$$

We can then evaluate the asymptotic values of these terms as follows: For $0 \leq i, j \leq k - 1$ the asymptotic value of the $(i+2, j+2)^{th}$ $d \times d$ block of the matrix $(\bar{Q}_{k-1,\ell}^-)^T \bar{Q}_{k\ell}^+$ is

$$\lim_{N_\ell \to \infty} \frac{1}{N_\ell} \left[ \bar{Q}_{k-1,\ell}^+ \right]_{i+2,j+2} = \lim_{N_\ell \to \infty} \frac{1}{N_\ell} \left( q_{k\ell}^+ \right)^T q_{i\ell}^+ = \lim_{N_\ell \to \infty} \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} \left[ q_{i\ell}^+ \right]_n \left[ q_{k\ell}^+ \right]_n = \frac{1}{N_\ell} \mathbb{E} \left[ q_{i\ell}^+ q_{k\ell}^+ T_q \right],$$

where (a) follows since the $(i+2)^{th}$ column block of $\bar{Q}_{k-1,\ell}^+$ is $q_{i\ell}^+$, and (b) follows due to the empirical assumption in (40). Also, since the first column block of $\bar{Q}_{k-1,\ell}^+$ is $q_0^+$, we obtain that

$$\lim_{N_\ell \to \infty} \frac{1}{N_\ell} \left( \bar{Q}_{k-1,\ell}^+ \right)^T \bar{Q}_{k-1,\ell}^- = \mathbf{R}_{k-1,\ell}^+ \quad \text{and} \quad \lim_{N_\ell \to \infty} \frac{1}{N_\ell} \left( \bar{Q}_{k\ell}^- \right)^T \bar{Q}_{k\ell}^+ = \mathbf{R}_{k\ell}^- \quad (52)$$

where $\mathbf{R}_{k-1,\ell}^+$ is the covariance matrix of $\left[ Q_0^+ Q_1^- \ldots Q_{k-1}^- \right]$, and $\mathbf{R}_{k\ell}^-$ is the covariance matrix of $\left[ Q_1^- Q_2^- \ldots Q_{k\ell}^- \right]$. For the matrix $(\bar{Q}_{k-1,\ell}^+)^T \bar{Q}_{k\ell}^+$, first observe that the limit of the divergence free condition (38) implies

$$\mathbb{E} \left[ \left( \partial_{q_{i\ell}}^+ \left( P_{i+1,\ell}^+ Q_{k\ell}^+ W_{i\ell}^T \right) \right)^T q_{k\ell}^+ \right] = \lim_{N_\ell \to \infty} \left( \mathbb{E} \left[ \partial_{q_{i\ell}}^+ \left( P_{i+1,\ell}^+ Q_{k\ell}^+ W_{i\ell}^T q_{k\ell}^+ \right) \right] \right) = 0,$$

for any $i$. Also, by the induction hypothesis $H_{k\ell}^+$,

$$\mathbb{E}(P_{i+1,\ell}^+ Q_{k\ell}^+) = 0, \quad \mathbb{E}(P_{i+1,\ell}^+ Q_{k\ell}^+) = 0, \quad (54)$$

for all $0 \leq i, j \leq k$. Therefore using (42), the cross-terms $\mathbb{E}(Q_{i\ell}^+ Q_{k\ell}^+)$ are given by

$$\mathbb{E}(f_{i\ell}^+ (P_{i+1,\ell}^+ P_{i,\ell+1}^- Q_{i,\ell+1}^+ W_{i\ell}^T \bar{Q}_{i\ell}^-)^T q_{k\ell}^+)$$

$$(a) = \mathbb{E} \left[ \left( \partial_{P_{i+1,\ell}^+} \left( P_{i+1,\ell}^+ P_{i,\ell+1}^- Q_{i,\ell+1}^+ W_{i\ell}^T \bar{Q}_{i\ell}^- \right) \right)^T q_{k\ell}^+ \right] \mathbb{E}(P_{i+1,\ell}^+ T_q)$$

$$+ \mathbb{E} \left[ \left( \partial_{P_{i,\ell+1}^-} \left( P_{i+1,\ell}^+ P_{i,\ell+1}^- Q_{i,\ell+1}^+ W_{i\ell}^T \bar{Q}_{i\ell}^- \right) \right)^T q_{k\ell}^+ \right] \mathbb{E}(P_{i,\ell+1}^- T_q)$$

$$+ \mathbb{E} \left[ \left( \partial_{Q_{i,\ell+1}^+} \left( P_{i+1,\ell}^+ P_{i,\ell+1}^- Q_{i,\ell+1}^+ W_{i\ell}^T \bar{Q}_{i\ell}^- \right) \right)^T q_{k\ell}^+ \right] \mathbb{E}(P_{i+1,\ell}^+ T_q)$$

(b) follows from a multivariate version of Stein’s Lemma [49, eqn.(2)]; and (b) follows from (53), and (54). Consequently,

$$\lim_{N_\ell \to \infty} \frac{1}{N_\ell} B_{k\ell}^T B_{k \ell} = \left[ \mathbf{R}_{k-1,\ell}^+ \right]$$

where $B_{k\ell}^T B_{k \ell} = \mathbb{E}(Q_{i\ell}^+ Q_{k\ell}^+)$ is the matrix of correlations. We again have $0$ in the second term because $\mathbb{E}(Q_{i\ell}^+ Q_{k\ell}^+) = 0$ for all $0 \leq i, j \leq k$. Hence we have

$$\lim_{N_\ell \to \infty} \frac{1}{N_\ell} B_{k\ell}^T B_{k \ell}^{-1} B_{k\ell} q_{k\ell}^+ = \left[ \beta_{k\ell}^+ \right] \left[ \beta_{k\ell}^+ \right] \mathbf{0}$$

(57)

Therefore, $p_{k\ell}^{+\text{det}}$ equals

$$A_{k\ell}(B_{k\ell}^T B_{k\ell})^{-1} B_{k\ell} q_{k\ell}^+ = \left[ \bar{P}_{k-1,\ell}^+ \bar{P}_{k,\ell}^- \right] \left[ \beta_{k\ell}^+ \right] + O \left( \frac{1}{\sqrt{N_\ell}} \right),$$

where $\beta_{k\ell}^+$ and $\beta_{k\ell}^+$ are $d \times d$ block matrices of $\beta_{k\ell}^+$ and the term $O(\frac{1}{\sqrt{N_\ell}})$ means a matrix sequence, $\varphi(N) \in \mathbb{R}^{N_\ell}$ such that $\lim_{N_\ell \to \infty} \frac{1}{N_\ell} ||\varphi(N)||^2 = 0$. A continuity argument then shows the empirical convergence (50).

Lemma 5. Under the induction hypothesis, the components of the “random” term $p_{k\ell}^{+\text{ran}}$ along with the components of the vectors in $\bar{v}_{k\ell}$ almost surely converge empirically. The components of $p_{k\ell}^{+\text{ran}}$ converge as

$$p_{k\ell}^{+\text{ran}} \Rightarrow U_{k\ell},$$

(59)

where $U_{k\ell}$ is a zero mean Gaussian random vector in $\mathbb{R}^{d \times d}$ independent of the limiting random variables corresponding to the variables in $\bar{v}_{k\ell}$.

Proof. The proof is identical to that of [26, Lemmas 7.8].

We are now ready to prove Lemma 3.

Proof of Lemma 3. Using the partition (49a) and Lemmas 4 and 5, we see that the components of the vector sequences in $\bar{v}_{k\ell}$ along with $p_{k\ell}^{+\text{ran}}$ almost surely converge jointly empirically, where the components of $p_{k\ell}^{+\text{ran}}$ have the limit

$$p_{k\ell} = p_{k\ell}^{\text{det}} + p_{k\ell}^{+\text{ran}} = \frac{p_{k\ell}}{\sqrt{\beta_{k\ell}^+} P_{k\ell}^+} + \sum_{i=0}^{k-1} p_{i+1,\ell}^+ \beta_{k\ell}^+ + U_{k\ell} =: P_{k\ell}^+.$$

Note that the above Wasserstein-2 convergence can be shown using the same arguments involved in showing that if $X_N \Rightarrow d \Rightarrow X$, and $Y_N \Rightarrow d \Rightarrow c$, then $(X_N, Y_N) \Rightarrow d \Rightarrow (X, c), |F|$ for some constant $c$ and sigma-algebra $F$.

We first establish the Gaussianity of $P_{k\ell}^+$. Observe that by the induction hypothesis, $H_{k,\ell+1}$ holds whereby $(P_0^+, P_1^+, \ldots, P_{k-1,\ell}^+, Q_{0,\ell+1}^- \ldots, Q_{k,\ell+1}^-)$ is jointly Gaussian. Since $U_{k\ell}$ is Gaussian and independent of
where (a) follows from (60) and, in (b), we used the fact that \( K \) is jointly Gaussian.

We now need to prove the correlations of this jointly Gaussian random vector are as claimed by \( H_{k,\ell+1}^+ \). Since \( H_{k,\ell+1}^+ \) is true, we know that (41) is true for all \( i = 0, \ldots, k-1 \) and \( j = 0, \ldots, k \) and \( \ell = \ell + 1 \). Hence, we need only to prove the additional identity for \( i = k \), namely the equations:

\[
\text{Cov}(P_{\ell}^0, P_{k,\ell}^+)^2 = K_{k,\ell}^+ \quad \text{and} \quad \mathbb{E}(P_{k,\ell}^+ Q_{\ell,\ell+1}^-) = 0.
\]

First observe that

\[
\mathbb{E}(P_{k,\ell}^+ P_{k,\ell}^+) = \frac{1}{N} \mathbb{E} \left( \mathbf{1}_k \right) \mathbf{1}_k^T \rightarrow \mathbf{1}_k \mathbf{1}_k^T = K_{k,\ell}^+ \quad \text{as} \quad \ell \rightarrow \infty.
\]

We need only to prove the correlations of this jointly Gaussian random vector are as claimed by \( H_{k,\ell+1}^+ \). Since \( H_{k,\ell+1}^+ \) is true, we know that (41) is true for all \( i = 0, \ldots, k-1 \) and \( j = 0, \ldots, k \), and \( \ell = \ell + 1 \). Hence, we need only to prove the additional identity for \( i = k \), namely the equations:

\[
\text{Cov}(P_{\ell}^0, P_{k,\ell}^+)^2 = K_{k,\ell}^+ \quad \text{and} \quad \mathbb{E}(P_{k,\ell}^+ Q_{\ell,\ell+1}^-) = 0.
\]

where (a) follows from the fact that the rows of \( P_{k,\ell}^+ \) converge empirically to \( P_{k,\ell}^+ \); (b) follows from line 20 in Algorithm 3 and the fact that \( V_{\ell} \) is orthogonal; and (c) follows from the fact that the rows of \( Q_{\ell,\ell+1}^- \) converge empirically to \( Q_{\ell,\ell+1}^- \) from hypothesis \( H_{k,\ell}^+ \). Since \( P_{\ell}^0 = V_{\ell} Q_{\ell}^0 \), we similarly obtain that

\[
\mathbb{E}(P_{\ell}^0 P_{\ell}^0) = \mathbb{E}(Q_{\ell}^0 Q_{\ell}^0), \quad \mathbb{E}(P_{\ell}^0 P_{\ell}^0) = \mathbb{E}(Q_{\ell}^0 Q_{\ell}^0),
\]

from which we conclude

\[
\text{Cov}(P_{\ell}^0, P_{k,\ell}^+)^2 = \text{Cov}(Q_{\ell}^0, Q_{k,\ell}^+) = : K_{k,\ell}^+.
\]

where the last step follows from the definition of \( K_{k,\ell}^+ \) in line 20 of Algorithm 4. Finally, we observe that for \( 0 \leq j \leq k \)

\[
\mathbb{E}(P_{\ell}^+ Q_{\ell,\ell+1}^-) = 0, \quad \text{where (a) follows from (60) and, in (b), we used the fact that}
\]

\[
\mathbb{E}(P_{\ell}^0 Q_{\ell,\ell+1}^-) = 0, \quad \text{and (c) follows from the fact that the rows of}
\]

\[
Q_{\ell,\ell+1}^- \quad \text{converge empirically to} \quad Q_{\ell,\ell+1}^- \quad \text{from hypothesis} \quad H_{k,\ell}^+.
\]

Thus, with (61) and (62), we have proven all the correlations in (41) corresponding to \( H_{k,\ell+1}^+ \).

Next, we prove the convergence of the parameter lists \( T_{k,\ell+1}^+ \) to \( T_{k,\ell+1}^+ \). Since \( T_{k,\ell}^- \to T_{k,\ell}^- \) due to hypothesis \( H_{k,\ell}^+ \), and \( T_{k,\ell+1}^+ \) is uniformly Lipschitz continuous, we have that

\[
\lim_{N \to \infty} T_{k,\ell+1}^+ \text{ converges almost surely as}
\]

\[
\lim_{N \to \infty} \left< \varphi_{k,\ell+1}^+(P_{\ell}^0, P_{k,\ell}^+, Q_{\ell,\ell+1}^+, W_{\ell,\ell+1}, T_{k,\ell}^+) \right> = \mathbb{E} \left[ \varphi_{k,\ell+1}^+(P_{\ell}^0, P_{k,\ell}^+, Q_{\ell,\ell+1}^+, W_{\ell,\ell+1}, T_{k,\ell}^+) \right] = \pi_{k,\ell+1}^+.
\]

which proves the convergence of the parameter lists stated in \( H_{k,\ell+1}^+ \). Finally, using (64), the empirical convergence of the matrix sequences \( P_{\ell}^0, P_{k,\ell}^+ \) and \( Q_{\ell,\ell+1}^- \) and the uniform Lipschitz continuity of the update function \( f_{k,\ell+1}(\cdot) \) we obtain that \( Q_{k,\ell+1}^+ \) equals

\[
f_{k,\ell+1}(P_{\ell}^0, P_{k,\ell}^+, Q_{\ell,\ell+1}^+, W_{\ell,\ell+1}, T_{k,\ell}^+) =: Q_{k,\ell+1}^+.
\]

An overview of the iterates in Algorithm 3 is depicted in (TOP) and (MIDDLE) of Figure 3. Theorem 2 shows that the rows of the iterates of Algorithm 3 converge empirically with 2\textsuperscript{nd} order moments to random variables defined in Algorithm 4. The random variables defined in Algo. 4 are depicted in Figure 3 (BOTTOM).
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