Probabilistic Federated Learning of Neural Networks Incorporated with Global Posterior Information

Peng Xiao, Samuel Cheng*, Senior Member, IEEE

Abstract—In federated learning, models trained on local clients are distilled into a global model. Due to the permutation invariance arises in neural networks, it is necessary to match the hidden neurons first when executing federated learning with neural networks. Through the Bayesian nonparametric framework, Probabilistic Federated Neural Matching (PFNM) matches and fuses local neural networks so as to adapt to varying global model size and the heterogeneity of the data. In this paper, we propose a new method which extends the PFNM with a Kullback-Leibler (KL) divergence over neural components product, in order to make inference exploiting posterior information in both local and global levels. We also show theoretically that The additional part can be seamlessly concatenated into the match-and-fuse progress. Through a series of simulations, it indicates that our new method outperforms popular state-of-the-art federated learning methods in both single communication round and additional communication rounds situation.

Index Terms—Fedrated Learning, Bayesian Nonparametric, KL-divergence, Neural Network.

1 INTRODUCTION

NOWADAYS, edge devices such as mobile phones, wearable devices, and vehicles have access to a wealth of data. Considering the inherently private attribute of the data and communication cost, pooling data from many devices at the data center, and conducting centralized training is far from ideal. Thus, federated learning (FL), in which a model is learned from siloed data without centralized together, is proposed to tackle this challenge.

Federated learning is a learning paradigm where local clients train models with their local datasets and then locally trained models will be gathered and fused into a shared global model. As one of the standard aggregation methods, FedAvg [11] creates the global model by weighted averaging parameters of local models with weights proportional to sizes of the local datasets in a coordinate-wise manner. However, this coordinate-wise averaging in FedAvg was shown to be not-optimum [21] and the performance of FedAve grows can also deteriorate significantly as statistical heterogeneity in non-i.i.d (Independent and Identically Distributed) data increases [10]. To address the weakness of coordinate-wise averaging, one can leverage an important observation that the ordering of neurons in the hidden layers of the neural network (NN) is permutation invariant. Consequently, one can reformulate federated learning as an adaptive matching problem that groups the same general type of neurons across local NNs before aggregating them into a global entirety [22].

Probabilistic Federated Neural Matching (PFNM) [22] developed Bayesian nonparametric model in order to match and combine NNs across data sources. They treat the neurons of locally trained NNs as noisy realizations of latent global neurons and formally characterize the generative process through a Beta-Bernoulli process (BBP) [18]. The matching is then governed by maximum a posterior (MAP) of the BBP which allows local neurons to either match existing global neurons or create new global neurons if existing ones are poor matches.

Recently, [2] proposes a method to fuse a model’s posterior distribution learned from heterogeneous datasets. The authors pose the problem of recovering a global distribution as that of minimizing the sum of Kullback-Leibler (KL) divergence from the local distributions while preserving the inherent permutation invariance of components. Such a fusion approach demonstrates effectiveness for applications like motion capture analysis and topic modeling, where a global posterior is required. In this paper, inspired by work in [2], we extend the MAP inference in PFNM through an additional KL divergence penalty that incorporates local neuron information under the BBP. Doing so allows an inference to exploit the posterior information at both the local and global levels. We call this new probabilistic federated learning framework Global Posterior Incorporated Federated Neural Matching (GPI-FNM) and theoretically prove that the additional KL-divergence in the GPI-FNM objective function can be seamlessly concatenated with PFNM during the matching process without extra time complexity. And through a series of simulated experiments on both MNIST and CIFAR10 datasets, we demonstrate GPI-FNM outperforms some federated learning baselines, including PFNM.

The remainder of the paper is organized as follows. We briefly introduce some backgrounds and related works in Section 2. The preliminaries and problem formulation are described in Section 3. We then present the proposed method in Section 4 and empirically show its performance.
in Section 5. Finally, Section 6 concludes our work and discusses some future works.

2 Background and Related Works

This section briefly reviews some basic mathematical tools required by our framework and some related works on Federated Learning.

2.1 Beta-Bernoulli Process and Indian Buffet Process

Denote \( Q \) as a random measure drawn from a Beta process: \( Q | \gamma_0, H \sim \text{BP}(1, \gamma_0 H) \), where \( \gamma_0 \) is the mass parameter, \( H \) is the base measure over some domain \( \Omega \) such that \( H(\Omega) = 1 \). One can show \( Q \) to be a discrete measure with \( Q = \sum_i q_i \delta_{\theta_i} \), which can be characterized by an infinitely countable set of (weight, atom) pairs \( (q_i, \theta_i) \in [0, 1] \times \Omega \). The atoms \( \theta_i \) can be drawn i.i.d from \( H \) and the weights \( \{q_i\}_{i=1}^\infty \) can be generated via a stick-breaking process [17]: \( q_i \sim \text{Beta}(\gamma_0, 1) \), \( q_i = \prod_{g=1}^\infty g_g \). Then subsets of atoms in the random measure \( Q \) can be picked via a Bernoulli process. That is to say, each subset \( T_s \) for \( s = 1, \cdots, S \) can be distributed via a Bernoulli process with base measure \( Q: T_s|Q \sim \text{BeP}(Q) \). Hence, it can also show subset \( T_s \) as a discrete measure \( T_s := \sum_i a_{si} \theta_i \), which is formed by pairs \( (a_{si}, \theta_i) \in [0, 1] \times \Omega \), where \( a_{si} | q_i \sim \text{Bernoulli}(q_i) \). That is, \( \theta_i \) belongs to subset \( T_s \). It regards such collection of subsets as being distributed by a Beta-Bernoulli process [18].

The Indian buffet process (IBP) specifies distribution on sparse binary matrices [6]. IBP involves a metaphor of a sequence of customers tasting dishes in an infinite buffet: the first customer tastes Poisson(\( \gamma_0 \)) dishes, every subsequent customer tastes the dishes that are previously selected with probability \( n_s / n_i \), where \( n_i = \sum_{s=1}^{S-1} a_{si} \), and then tastes Poisson(\( \gamma_0 / s \)) new dishes. Marginalizing over Beta Process distributed \( Q \) above will induce dependencies among subsets and recover the predictive distribution \( T_S | T_1, \cdots, T_{S-1} \sim \text{BeP}(H S_0 + \sum_{g=1}^\infty g_g \delta_{\theta_g}) \) (dependency on \( S \) is suppressed in the notation for simplicity). That is equivalent to the IBP.

2.2 Related Works

Distributed deep learning has been developed in the past decade [4, 9, 23, 9, 15]. As privacy concerns emerged and, edge devices such as phones, wearable devices, and vehicles grow both in power and computation, each device preferably learns independent local models through their own data instead of collecting them together in a data center. Thus federated learning has been advocated as an important learning paradigm.

As an emerging field, federated learning has gathered interest in both theory [2, 16] and application [1, 5, 20]. And a lot of optimization methods that are customized for federated learning have emerged. In particular, federated learning is treated as a multi-task learning problem and exploited through the convexity of the support vector machine (SVM) in [16]. Still, such a method is not generalized to the non-convex problem like neural networks considered in our work. In the non-convex setting, FedAvg [11] proposes a strategy that averages each local updates to learn a federated global model. FedeProx [10] adds a proximal term to the client cost functions to keep local updates close to the global model to ensure convergence. Agnostic Federated Learning (AFL) [12], as another variant of FedAvg, optimizes a centralized distribution to maximize the performance of the worst performing client. However, due to the inherent permutation invariance of neural network (NN) parameters, such averaging-like methods may have drastic detrimental effects on the averaged model’s performance and adds significantly to the communication burden.

PFNM [22] emphasizes training and aggregating NNs. It developed a Bayesian nonparametric model for federated learning and matched the neurons across NNs before aggregating them. It also is extended in modern architecture like CNNs and LSTMs [19]. However, their approach only makes a point estimate of local posterior and precludes using full information like covariances. Inspired by the model fusion work in [2], we extend the original PFNM by incorporating global posterior information during the matching progress. The proposed new method is theoretically proved to inherit non-parametric nature and shown to have better performance compared to PFNM through experiments.

3 Preliminaries and Problem Formulation

This section introduces the preliminary notations of federated learning in neural networks and the permutation invariance classes of neural networks. And then, we will formulate the adaptive matched aggregating problem of federated neurons.

3.1 Preliminaries

Suppose there are \( S \) fully connected (FC) NNs with one hidden layer trained from different datasets: \( f_s(x) = \text{softmax}(\sigma(W_s(0)x)) \), for \( s = 1, \cdots, S \) (without loss of generality, biases are omitted to simplify notation), where \( \sigma(\cdot) \) is the non-linearity, \( W_s(0) \in \mathbb{R}^{D \times J_s} \), \( W_s(1) \in \mathbb{R}^{K \times J} \) be the weights; \( D \) is the input dimension, \( J_s \) is the number of neurons on the hidden layer of \( s \)-th NN, and \( K \) is the output dimension (i.e., number of classes). In federated learning, given the collection of weights \( \{W_s^{(0)}, W_s^{(1)}\}_{s=1}^S \), we want to learn a global neural network with weights \( \Theta(0) \in \mathbb{R}^{D \times J}, \Theta(1) \in \mathbb{R}^{K \times J} \), where \( J \ll \sum_{s=1}^S J_s \) is an inferred variable denotes the number of hidden neurons of the global network.

3.2 Permutation Invariance of Neural Network

Expanding the preceding expression of a FCNN: \( f_s(x) = \sum_{j=1}^{J_s} \text{softmax}(\sigma(W_s(0)x)W_s^{(1)})) \), where \( j \) and \( j' \) denote \( j \)-th row and \( j' \)-th column correspondingly. Summation is a permutation invariant operation, thus for any permutation \( \tau(1, \cdots, J_s) \) of the \( s \)-th NN reordering columns of \( W_s^{(0)} \) and rows of \( W_s^{(1)} \) has no impact on the outputs \( f_s(x) \) for arbitrary value of \( x \).

Because the \( S \) NNs are trained through data with the same general type (not necessarily homogeneous), it could assume that different NNs at least share some neurons (i.e., feature extractors) that serve the same purpose. However, due to the inherent permutation invariance discussed above,
3.3 Adaptive Matched Aggregation Formulation

Here we formulate a practical notion of federated local neurons aggregation under the permutation invariance and describe how to solve iteratively. Let \( w_{sj} \) be the \( j \)th neuron learned on dataset \( s, \theta_i \) denote the \( i \)th neuron in the global model \( w_{sj}, \theta_i \in \mathbb{R}^{D+K} \) can be seen as a concatenated vector of weights. \( c(\cdot, \cdot) \) could be an appropriate function showing similarity between local and global neuron. The solution to the following optimization problem is the required matching assignments:

\[
\min_{\{A^s\}} \sum_{i=1}^{J} \min_{\theta_i} \sum_{s=1}^{S} \sum_{j=1}^{J_s} A^s_{i,j} c(w_{sj}, \theta_i)
\]

\[
s.t. \sum_i A^s_{i,j} = 1 \quad \forall s, j; \sum_j A^s_{i,j} \leq 1 \quad \forall s, i; A^s_{i,j} \in \{0, 1\}.
\]

The \( \{A^s\}_{s=1}^S \) are the collection of assignment variables of each dataset \( s \), where \( A^s_{i,j} = 1 \) implies the local neuron \( w_{sj} \) matched with global neuron \( \theta_i \) and vice versa. After assignments come out, the global model \( \{\theta_i\} = \arg\min_{\theta_i} \sum_{s,j} A^s_{i,j} c(w_{sj}, \theta_i) \) will be typically constructed via a closed form. The equality constraint implies that neurons in one client are a subset of aggregated global. The inequality constraint indicates that neurons across clients may overlap only partially because of the data heterogeneity in Federated Learning. Thus the size of constructed global model \( J \) satisfying \( \max_{s} J_s \leq J \leq \sum_s J_s \) and is adaptive during the matching process.

The assignments can be solved and global model can be constructed by an iterative approach: denote \(-s'\) as "all but \( s'\)," fixing assignments \( \{A^s_{i,j}\}_{i,j,s\neq s'} \) we find optimal assignments \( \{A^s_{i,j}\}_{i,j,s} \) corresponding to dataset \( s' \) and iterating over remaining datasets. At each iteration, given current estimates of \( \{A^s_{i,j}\}_{i,j,s\neq s'} \), we find a corresponding matched aggregating global model \( \{\theta_i\} = \arg\min_{\theta_i} \sum_{s} A^s_{i,j} c(w_{sj}, \theta_i) \) via the closed form expression, \( J_{s'} = \max \{i : A^s_{i,j} = 1, \text{for } s \in -s', j = 1, \ldots, J_s \} \) denote number of active global neurons outside of \( s' \). When matching neurons \( \{w_{sj}\}_{J_{s'}=1}^J \) of dataset \( s' \) to this global model, due to data heterogeneity, local model \( s' \) may have neurons not present in current global model built from other local models. Therefore, if one local neuron’s optimal match has cost larger than some threshold value \( \epsilon \), the corresponding local one should be treated as a new global neuron. It also wants a modest size global model and therefore penalizes its size with some increasing function \( f(J') \), \( J' \) denotes the new model size. This intuition can be formalized in the following extended linear sum assignment problem:

\[
\min_{\{A^s_{i,j}\}} \sum_{i=1}^{J_{s'}+J_{s'}} \sum_{j=1}^{J_{s'}} A^s_{i,j} C^s_{i,j}
\]

\[
s.t. \sum_i A^s_{i,j} = 1, \sum_j A^s_{i,j} \in \{0, 1\} \quad \text{and} \quad C^s_{i,j} = \begin{cases} c(w_{sj}, \theta_i), & i \leq J_{s'}, \\ \epsilon + f(i), & J_{s'} < i \leq J_{s'} + J_{s'}. \end{cases}
\]

(2) can be solved by Hungarian algorithm [8]. The size of the new global model is then \( J' = \max \{i : A^s_{i,j} = 1, j = 1, \ldots, J_s \} \) and thus \( J_{s'} \leq J' \leq J_{s'} + J_s \). The key step of whole matching process is the derivation of assignment cost specifications \( \{C^s_{i,j}\}_{i,j} \). The overall matched aggregation procedure is summarized in Figure 1.

4 Federated Neural Matching: Methods

In this section we first review the PFNM [22] and then introduce our global posterior incorporated version — GPI-FNM. We also port the proposed framework into deep neural networks and networks with multiple communication rounds.

4.1 PFNM

Beta-Bernoulli process based model PFNM models the generative process of observed local neurons via a Beta-Bernoulli process [22]. In there, global atoms (hidden layer neurons) are drawn from a Beta process prior with a base measure \( H \) and mass parameter \( \gamma_0, Q = \sum q_i \delta_{\theta_i} \). \( H \) is chosen as multi-Gaussian distribution \( H = N(\mu_0, \Sigma_0) \) with \( \mu_0 \in \mathbb{R}^{D+K} \) and diagonal \( \Sigma_0 \).

Local atoms are observed as noisy measurements of subsets of global atoms \( w_{s|T_s} \sim N(T_s, \Sigma_s) \) for \( s = 1, \ldots, S; j = 1, \ldots, J_s, J_s := card(T_s) \). The subset \( T_s \) is selected via the Bernoulli process: \( T_s := \sum a_s \delta_{\theta_i} \) where \( a_s \sim \text{Bern}(q_i) \forall i. T_s \) is supported by atoms \( \{\theta_i : a_s = 1, i = 1, 2, \ldots\} \) represent the identities of the atoms (neurons) used by subset \( s \). Under this model, there is a one-to-one correspondence between \( \{a_s\}_{s=1}^S \) and assignment variables \( \{A^s\}_{s=1}^S \) to be inferred, where \( A^s_{i,j} = 1 \) implies \( T_s \).

Maximum a posterior estimation To formulate the objective function related to (1), PFNM maximizes a posterior estimation (i.e., minimizing the negative one) of global neurons for the model presented above:

\[
\max_{\{\theta_i\}, \{A^s\}} P(\{\theta_i\}, \{A^s\}\{w_{sj}\})
\]

\[
\times P(\{w_{sj}\}\{\theta_i\}, \{A^s\})P(\{A^s\})P(\{\theta_i\}),
\]

(3) by taking negative logarithm it can obtain:

\[
\min_{\{\theta_i\}, \{A^s\}} - \sum_i \left( \sum_{s,j} A^s_{i,j} \log(p(w_{sj} | \theta_i)) + \log(p(\theta_i)) \right)
\]

\[ - \log(P(\{A^s\})) \]

(4) where \( w_{sj} \sim \theta_i \) here denotes \( w_{sj} \) generated with mean \( \theta_i \). \( P(\{A^s\}) \) is interpreted by IBP and demonstrated in the appendix. Given \( \{A^s\}_{s=1}^S \), the closed-form expression of
Fig. 1. The matching progress of three local NNs via Federated Neural matched aggregation. Colored nodes in here indicate hidden neurons; the same color hidden neurons have been matched. In here, hidden neurons in each of $S$ NNs can be treated as weight vectors ($\in \mathbb{R}^{d+K}$) referencing both input ($\in \mathbb{R}^d$) and output ($\in \mathbb{R}^K$) layer. These weight vectors will then be used to form a cost matrix corresponding in (6), which is used by the Hungarian algorithm to do the matching. Finally, the matched neurons are aggregated to form the global model.

$\{\theta_i\}$ can be estimated according to the Gaussian-Gaussian conjugacy:

$$\hat{\theta}_i = \frac{\mu_0}{\sigma_0^2} + \frac{\sum_{s,j} A_{i,j}^s w_{s,j} / \sigma_s^2}{1 / \sigma_0^2 + \sum_{s,j} A_{i,j}^s / \sigma_s^2} \quad \text{for } i = 1, \ldots, J, \quad (5)$$

where for simplicity assume $\Sigma_0 = I\sigma_0^2$ and $\Sigma_s = I\sigma_s^2$. Using this fact it has the following proposition to obtain the assignment cost $\{C_{i,l}\}_{i,l}$ corresponding in (2):

**Proposition 1.** The assignment cost specification for finding $\{A_{i,l}\}$ corresponding to objective (4) is

$$C_{i,l} = \begin{cases} 
\frac{||\mu_0 + \sum_{s \neq s'} A^s_{i,j} \mu_{s,j}||^2}{\sigma_0^2 + \sum_{s \neq s'} A^s_{i,j} / \sigma_s^2} + \frac{||\mu_0 + \sum_{s \neq s'} A^s_{i,j} \mu_{s,j}||^2}{\sigma_0^2 + \sum_{s \neq s'} A^s_{i,j} / \sigma_s^2} 
- 2 \log \frac{\mu_{s,j}}{\mu_{s,j} - \sigma_{s,j}^2}, & i \leq J_s' \\
- \frac{||\mu_0 + \sum_{s \neq s'} A^s_{i,j} \mu_{s,j}||^2}{\sigma_0^2 + \sum_{s \neq s'} A^s_{i,j} / \sigma_s^2} 
+ \frac{||\mu_0 + \sum_{s \neq s'} A^s_{i,j} \mu_{s,j}||^2}{\sigma_0^2 + \sum_{s \neq s'} A^s_{i,j} / \sigma_s^2} 
+ 2 \log \frac{\mu_{s,j} - \sigma_{s,j}^2}{\mu_{s,j}}, & J_s' < i \leq J_s + J_s', 
\end{cases}$$

where $n_{s'} = \sum_{s \neq s'} A^s_{i,j}$ denote number of times client neurons were assigned to global neuron $i$ outside of $s'$. Proof can be found in [22] and also be referred in the appendix.

### 4.2 GPI-FNM

When formulating the matching objective function, MAP exploits information about point estimate of latent variables. The similarity is the posterior probability of $w_{s,j}$ generated from a Gaussian distribution with mean $\theta_i$. That means all information applied for inferring is between a pair of neural components. Inspired by work in [22], it can also pose the problem of recovering a global model as that of minimizing a divergence to the local models. Specifically, by minimizing the following KL divergence $\text{KL}(\cdot||\cdot)$ between the products of the global and local neural components:

$$\min_{\{\theta_i\},\{A_{s,j}\}} \sum_s \text{KL} \left( \prod_j p(\sum_i A_{i,j}^s \theta_i) || \prod_j p(w_{s,j}) \right), \quad (7)$$

it is asking for the choice of global neuron $\theta_i$ as well as an assignment for each dataset telling how to put $\theta_i$ and $w_{s,j}$ in correspondence at a global level, where inner sum $\sum_i A_{i,j}^s \theta_i$ denotes the global neuron that match the local neuron. When treating (7) as an additional term of (4):

$$\min_{\{\theta_i\},\{A_{s,j}\}} \sum_i \left( \sum_{s,j} A_{i,j}^s \log(p(w_{s,j} | \theta_i)) \right) + \log(p(\theta_i)) - \log(P(\{A_{s,j}\}))$$

$$+ \sum_s \text{KL} \left( \prod_j p(\sum_i A_{i,j}^s \theta_i) || \prod_j p(w_{s,j}) \right), \quad (8)$$

it means incorporating original PFNM with global posterior information. We call this global posterior incorporated federated neural matching (GPI-FNM). Coefficient $\varepsilon$ adjusts the ratio of information quantity between local level and global level. In the remaining part, we mainly focus on the global part of (8), and prove (7) can also be derived as a linear sum assignment problem like the form of (6).

Decomposing over product distributions in $\text{KL}(\cdot||\cdot)$ and exploiting binary constraints in our problems, it allows us to write (7) as

$$\min_{\{\theta_i\},\{A_{s,j}\}} \sum_i \sum_{s,j} A_{i,j}^s \text{KL}(p(\theta_i) || p(w_{s,j})), \quad (9)$$
acording to the KL divergence between two multi-Gaussian distributions, we obtain:

\[
\min_{\{\theta_i\}, \{A_{s}^j\}} \frac{1}{2} \sum_{i,j} A_{s,i,j}^2 \left( (D + K) \left( \frac{\sigma_0^2}{\sigma_s^2} - 1 + \log \frac{\sigma_s^2}{\sigma_0^2} \right) + \frac{||\theta_i - \mu_0||^2}{\sigma_s^2} \right) + \frac{||\theta_i - \mu_0||^2}{\sigma_s^2}.
\]

For the iterative optimizing procedure, we have the following proposition where (7) arrive at a linear sum assignment form like \( \sum_i \sum_j A_{s,i,j}^2 \theta_{i,j} \):

**Proposition 2.** The assignment cost specification for finding \( A_{s}^j \) corresponding to (7) is \( C_{s,j} = \)

\[
\sum_{j \in J_{s,j}} \sum_{i \in J_{s,j}} \left( \frac{||w_{s,i,j} - \mu_0||^2}{\sigma_{s,j}^2} + \frac{\text{Tr}(s_{s,j}^2)}{\sigma_{s,j}^2} \right),
\]

where \( J_{s,j} = \{ j : s_{s,j}^2 \neq 0 \} \), \( 1 \leq i \leq |J_{s,j}| \).

**Proof.** Combine (10) with (5), it can be optimized with respect only to \( \{A_{s}^j\}_{s=1}^S \).

We now consider the first part of (12). We partition it between \( i = 1, \cdots, J_{s,j} \) and \( i = J_{s,j} + 1, \cdots, J_{s,j} + J_{s,j}' \), and since we are solving for \( A_{s}^j \), we can subtract terms independent of \( A_{s}^j \) (we use \( \equiv \) to say that two objective functions are equivalent up to terms independent of the interested variables):

\[
\sum_{i=1}^{J_{s,j}} \sum_{j \in J_{s,j}} \sum_{s \in J_{s,j}} A_{s,i,j}^2 \left( \frac{||w_{s,i,j} - \mu_0||^2}{\sigma_{s,j}^2} + \frac{\text{Tr}(s_{s,j}^2)}{\sigma_{s,j}^2} \right) + (D + K) \left( \frac{\sigma_0^2}{\sigma_s^2} - 1 + \log \frac{\sigma_s^2}{\sigma_0^2} \right).
\]

Then we consider the second term of (12). By subtracting terms independent of \( B_{s}^j \) it has:

\[
\sum_{j=1}^{J_{s,j}} \sum_{i \in J_{s,j}} \sum_{s \in J_{s,j}} A_{s,i,j}^2 \left( \frac{||w_{s,i,j} - \mu_0||^2}{\sigma_{s,j}^2} + \frac{\text{Tr}(s_{s,j}^2)}{\sigma_{s,j}^2} \right) + (D + K) \left( \frac{\sigma_0^2}{\sigma_s^2} - 1 + \log \frac{\sigma_s^2}{\sigma_0^2} \right).
\]

Because (15) is only varied by \( s' \), that means it adds equal cost in each item of \( C_{s,j}^j \), thus we can ignore it in the cost specification. From what has been discussed above, we obtain the assignment cost specification.

**GPI-FNM for Multilayer Neural Networks** As the same with PFNM [22], we can also naturally extend GPI-FNM to deep neural networks from outputs back to inputs (top-down). Denote \( L \) as the number of hidden layers and \( J^l \)
Algorithm 1 GPI-FNM

Input:
- Collected local weights \( w_{sj} \) from \( S \) clients;

Output:
- New constructed global model \( \{ \theta_i \} \);
1. Form each assignment cost matrix via \( 6 + \epsilon 11 \);
2. Use Hungarian algorithm to compute matching assignments \( \{ A_i^{s}\}_{s=1}^S \);
3. List all resulting distinct global neurons and then apply \( 5 \) to infer associated global weights from all instances of global neurons across \( S \) datasets;
4. Aggregate the global neurons to construct the new global model.

Algorithm 2 Multilayer GPI-FNM

Input:
- Collected local multilayer weights \( w_{sli} \) of from \( S \) clients, the number of hidden layers \( L \);

Output:
- New constructed global model \( \{ \theta_i \} \);
1: \( l = L \);
2: while \( layers \ l > 2 \) do
3: Call GPI-FNM with weights dimension equal to \( J^{l+1} \) (since the weights connecting to lower layers are not be used here);
4: Form the global neuron layer \( l \) from output of step 3;
5: \( J^l = \text{card(}U_{s=1}^S S_{s=1}^S \text{)} \);
6: \( l = l - 1 \);
end while
7: Match bottom layer by calling GPI-FNM with weights dimension equal to \( J^2 + J^0 \) (weights connecting to both input layer and above layer);
8: Return the global assignments and aggregate a global multilayer model.

as the number of neurons on the \( l \)th layer. Then \( J^0 = D \) and \( J^{L+1} = K \) are the number of input and output (label) dimension respectively. From top to down, to prevent unbounded dimension base measures, the global atoms have to be considered vectors referencing outgoing weights from neuron rather than as weights forming a neuron as the situation in the single hidden layer model previously.

Starting from the top hidden layer \( l = L \), each layer can be modeled similarly as in the single-layer case. Each layer generates a collection of global atoms and then selects a subset of them via Beta-Bernoulli process construction. \( J^{l+1} \) denotes the number of neurons on the layer \( l + 1 \), and it controls the dimension of the atoms in layer \( l \).

It is worth noting that different from the single layer case, some of the dimensions of \( w_{sli} \in \mathbb{R}^{J^{l+1}} \) now should be set to 0, because these dimensions correspond to outgoing weights to neurons of layer \( l+1 \) not present on dataset \( s \), i.e., \( w_{sli} \rightleftharpoons 0 \) if \( a_{sli}^{l+1} = 0 \) for \( i = 1, \ldots, J^{l+1} \). We can understand the resulting model as follows. A globally connected neural network has \( J^l \) neurons on layer \( l \) and each partially connected neural network has \( J_{s}^l \) active neurons on layer \( l \), and the weights of the remaining \( J^l - J_{s}^l \) neurons are zero and have no effect locally. The details of GPI-FNM for multilayer NNs are summarized in Algorithm 2.

4.3 GPI-FNM with Additional Communications

In the preceding sections, we proposed GPI-FNM to aggregate local models in a single communication round. In fact, the number of communication rounds is a key factor required in federated learning to achieve an accurate global model. Typically, local models are trained for few epochs, and trained parameters will be sent to the server for updating the global model. Then local models are reinitialized with the global model parameters for the new round. Thus it is natural to extend our approach to additional communication rounds as follows.

Denote \( t \) as a communication round. We set \( w_{sli}^{t+1} = \sum i A_{sli}^{l+1} \theta_i^t \) to initialize local models at round \( t + 1 \). As mentioned in above \( \sum i A_{sli} = 1 \forall j = 1, \ldots, J_s, s = 1, \ldots, S \), hence a local model is initialized with a subset of the global model, the local model size \( J_s \) is kept constant across communication rounds (which also holds for the multilayer case). After updating the local models, we apply the matching algorithm to obtain a new global model. The size of the global model can change across communication rounds. When the global model be updated in the last communication round, we get the final global entirety.

5 Experimental Results

This section presents an empirical study of GPI-FNM and compares it with PFNM \([22]\), and FedAvg \([11]\). Our experiments are conducted over two standard datasets: MNIST and CIFAR-10. And the experiments below show that our framework can aggregate multiple NNs into an efficient global one with as few as a single communication round and improve performance with additional communications.

5.1 Setup

Here we consider two partition strategies to simulate a federated learning scenario: (a) homogeneous partition where the proportion of each of the \( K \) classes are approximately equal in each client; and (b) heterogeneous partition where the number of data points and class proportions in each client is unbalanced. In heterogeneous partition, we sample \( p_k \sim Dir_{S}(0.4) \) into \( S \) clients and allocating a \( p_{k,s} \) proportion of the instances of class \( k \) to client \( s \). And because of the small concentration parameter (0.4) of the Dirichlet distribution, some sampled batches may even not have any instances of certain classes. In each of the four combinations of partition strategy and dataset, we execute 10 trials to obtain mean and standard deviations of the performances.

Our method and baselines operate on the collection of neural network weights from all partitioned batches. We applied PyTorch \([13]\) to implement these networks and train them by the AMSGrad optimizer \([14]\) with default parameters. All parameter settings are summarized in Table 1.
and heterogeneous cases, especially in deeper architectures. That shows incorporating global posterior information can alleviate the degradation when the data are insufficient for training local models.

5.3 Simulation with Additional Communication

Limiting communication as few as to a single communication round may be required in some common scenarios. However, in some other situations where a limited amount of additional communications is allowable also frequently arise in practice. This subsection investigates federated learning of a two-layer neural network with $S = 15$ clients and up to fifteen communications under a homogeneous partition and up to thirty communications under a heterogeneous partition. We compare GPI-FNM using the communication procedure to PFNM and federated averaging.

The results are reported in Figure 4. We can see that the performance of all three methods improves with increasing communication rounds. The GPI-FNM outperforms PFNM and FedAvg in all scenarios given sufficient communications, and GPI-FNM achieves a target performance level faster than both PFNM and federated averaging. In addition to improved performance, GPI-FNM provides a more steady performance than PFNM and federated averaging. In CIFAR 10 experiments, the performance of PFNM and federated averaging are both a little unstable, even falling back a bit with increasing communication rounds, but the GPI-FNM can still perform at a good level.

6 Conclusion

This paper has proposed a new federated neural matching method that enhanced the PFNM by incorporating global posterior information. We empirically demonstrated the new method outperforms state-of-the-art algorithms for federated learning of neural networks. In future work, it is naturally of interest to also extend our modeling framework to modern architectures such as Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs), where PFNM has already been extended well. And the success of KL-divergence also suggests we likely can extend our algorithm to other divergences (e.g., Bregman divergence) other than KL-divergence using a similar formulation and algorithm.

Appendix A

Proof of Proposition 1 [22]

PFNM maximizes a posterior probability of the global atoms $\{\theta_i\}_{i=1}^S$ and assignments of observed neural network weight estimates to global atoms $\{A^s\}_{s=1}^S$. Given estimates of the client weights $\{w_{s,j}\}$ for $j = 1, \ldots, J_s$ and assignments of observed neural network weight estimates to global atoms $\{A^s\}_{s=1}^S$, it has:

$$
\max_{\{\theta_i\}, \{A^s\}} P(\{\theta_i\}, \{A^s\}|\{w_{s,j}\}) 
\propto P(\{w_{s,j}\}|\{\theta_i\}, \{A^s\}) P(\{A^s\}) P(\{\theta_i\}),$$

(16)

by taking negative natural logarithm it can obtain:

$$
\min_{\{\theta_i\}, \{A^s\}} - \sum_{i} \left( \sum_{s,j} A^s_{i,j} \log(p(w_{s,j} | \theta_i)) + \log(p(\theta_i)) \right) 
- \log(P(\{A^s\})),$$

(17)
expand probability function of multi-dimensional Gaussian distributions in (17), it obtains:

$$
\min_{\{\theta_i\}, \{A^s\}} \frac{1}{2} \sum_i \left( \frac{||\hat{\theta}_i - \mu_0||^2}{\sigma_0^2} + (D + K) \log(2\pi \sigma_0^2) + \sum_{s,j} A^s_{i,j} \frac{||w_{sj} - \hat{\theta}_i||^2}{\sigma_s^2} \right) - \log(P(\{A^s\})).
$$

We now consider the first part of (18). Through the closed-form expression of $\{\theta_i\}$ estimated according to the Gaussian-Gaussian conjugacy:

$$
\hat{\theta}_i = \frac{\mu_0/\sigma_0^2 + \sum_{s,j} A^s_{i,j} w_{sj}/\sigma_s^2}{1/\sigma_0^2 + \sum_{s,j} A^s_{i,j}/\sigma_s^2} \quad \text{for } i = 1, ..., J,
$$

where for simplicity assume $\Sigma_0 = I\sigma_0^2$ and $\Sigma_s = I\sigma_s^2$, we can now cast first part of (18) with respect only to $\{A^s\}_{s=1}^S$:

$$
\frac{1}{2} \sum_i \left( \frac{||\hat{\theta}_i - \mu_0||^2}{\sigma_0^2} + (D + K) \log(2\pi \sigma_0^2) + \sum_{s,j} A^s_{i,j} \frac{||w_{sj} - \hat{\theta}_i||^2}{\sigma_s^2} \right)
$$

$$
\approx \frac{1}{2} \sum_i \left( \langle \hat{\theta}_i, \hat{\theta}_i \rangle \left( \frac{1}{\sigma_0^2} + \sum_{s,j} A^s_{i,j}/\sigma_s^2 \right) + (D + K) \log(2\pi \sigma_0^2) - 2 \langle \hat{\theta}_i, \sum_{s,j} A^s_{i,j} w_{sj}/\sigma_s^2 \rangle \right)
$$

$$
= -\frac{1}{2} \sum_i \left( \frac{||\sum_{s,j} A^s_{i,j} w_{sj} - \mu_0||^2}{1/\sigma_0^2 + \sum_{s,j} A^s_{i,j}/\sigma_s^2} - (D + K) \log(2\pi \sigma_0^2) \right),
$$

(20) partition (20) between $i = 1, ..., J\_s'$ and $i = J\_s' + 1, ..., J\_s' + J\_s'$, and because it is now solving for $A^{s'}$, it...
can subtract terms independent of $A^s$:

\[
\sum_{i=1}^{J-\epsilon'} \sum_{j=1}^{J'} A^s_{i,j} \left( \frac{||A^s_{i,j}^T w_j - \mu_j||_2^2}{\sigma^2_j} + \sum_{s'\in s'\,j} A^s_{i,j}^T w_{s'} - \mu_0 \right) - \sum_{i=1}^{J-\epsilon'} \sum_{j=1}^{J'} A^s_{i,j} \left( \frac{||A^s_{i,j}^T w_j - \mu_j||_2^2}{\sigma^2_j} + \sum_{s'\in s'\,j} A^s_{i,j}^T w_{s'} - \mu_0 \right)
\]

\[
\sum_{i=J-\epsilon'+1}^{J-\epsilon'} \sum_{j=1}^{J'} A^s_{i,j} \left( \frac{||A^s_{i,j}^T w_j - \mu_j||_2^2}{\sigma^2_j} + \sum_{s'\in s'\,j} A^s_{i,j}^T w_{s'} - \mu_0 \right)
\]

Thus (21) can rewritten as a linear sum assignment problem:

\[
\sum_{i=1}^{J-\epsilon'} \sum_{j=1}^{J'} A^s_{i,j} \left( \frac{||A^s_{i,j}^T w_j - \mu_j||_2^2}{\sigma^2_j} + \sum_{s'\in s'\,j} A^s_{i,j}^T w_{s'} - \mu_0 \right)
\]

\[
- \sum_{i=1}^{J-\epsilon'} \sum_{j=1}^{J'} A^s_{i,j} \left( \frac{||A^s_{i,j}^T w_j - \mu_j||_2^2}{\sigma^2_j} + \sum_{s'\in s'\,j} A^s_{i,j}^T w_{s'} - \mu_0 \right)
\]

\[
+ \sum_{i=J-\epsilon'+1}^{J-\epsilon'} \sum_{j=1}^{J'} A^s_{i,j} \left( \frac{||A^s_{i,j}^T w_j - \mu_j||_2^2}{\sigma^2_j} + \sum_{s'\in s'\,j} A^s_{i,j}^T w_{s'} - \mu_0 \right).
\]

Then consider the second term of (18), by subtracting terms independent of $A^s$ it has:

\[
\log(P(A^{s'})) = \log(P(A^{s'} | A^{-s'})) + \log(P(A^{-s'})).
\]

First, it can ignore $\log(P(A^{-s'}))$ since now are optimizing for $A^{s'}$. Second, due to exchangeability of datasets (i.e. customers of the IBP), $A^{s'}$ can always be treated as the last customer of the IBP. Denote $n_i^{-s'} = \sum_{s'\in s'\,j} A^s_{i,j}$ as the number of times local weights were assigned to global atom...
Fig. 4. Federated learning with communications. Test accuracy as a function of number of communication rounds for $J = 15$ batches and two layer neural networks. GPI-FNM consistently outperforms strong competitors.

outside of group $s'$. Now it can obtain the following:

$$\log P(A_{s'} | A^{-s'}) \simeq$$

$$\sum_{i=1}^{J-s'} \left( \sum_{j=1}^{J-s'} A_{i,j}^{s'} \log \frac{n_{i-s'}}{S} + \left( 1 - \sum_{j=1}^{J-s'} A_{i,j}^{s'} \right) \log \frac{S - n_{i-s'}}{S} \right)$$

$$- \log \left( \sum_{i=J-s'+1}^{J} \sum_{j=1}^{J-s'} A_{i,j}^{s'} + \sum_{i=J-s'+1}^{J} \sum_{j=1}^{J} A_{i,j}^{s'} \right) \log \frac{\gamma_0 S}{J}.$$  \hspace{1cm} (24)

\[24\] thus can be rearranged as linear sum assignment problem:

$$\sum_{i=1}^{J-s'} \sum_{j=1}^{J-s'} A_{i,j}^{s'} \log \frac{n_{i-s'}}{S - n_{i-s'}}$$

$$+ \sum_{i=J-s'+1}^{J} \sum_{j=1}^{J} A_{i,j}^{s'} \left( \log \frac{\gamma_0 S}{J} - \log (i - J-s') \right).$$  \hspace{1cm} (25)

Combine (22) and (25), we arrive at the cost specification shown in (6) of the main text. That completes the proof of Proposition 1 in the main text.

REFERENCES

[1] Keith Bonawitz, Hubert Eichner, Wolfgang Grieskamp, Dzmitry Huba, Alex Ingerman, Vladimir Ivanov, Chloe Kiddon, Jakub Konečný, Stefano Mazzocchi, H Brendan McMahan, et al. Towards federated learning at scale: System design. arXiv preprint arXiv:1902.01046, 2019.

[2] Sebastian Claici, Mikhail Yurochkin, Soumya Ghosh, and Justin Solomon. Model fusion with kullback–leibler divergence. arXiv preprint arXiv:2007.06168, 2020.

[3] Jeffrey Dean, Greg Corrado, Rajat Monga, Kai Chen, Matthieu Devin, Mark Mao, Marc’aurelio Ranzato, Andrew Senior, Paul Tucker, Ke Yang, et al. Large scale distributed deep networks. In Advances in neural information processing systems, pages 1223–1231, 2012.

[4] Ofer Dekel, Ran Gilad-Bachrach, Ohad Shamir, and Lin Xiao. Optimal distributed online prediction using mini-batches. The Journal of Machine Learning Research, 13:165–202, 2012.

[5] Yujia Gao, Liang Liu, Binxuan Hu, Tianzi Lei, and Huadong Ma. Federated region-learning for environment sensing in edge computing system. IEEE Transactions on Network Science and Engineering, 2020.

[6] Zoubin Ghahramani and Thomas L Griffiths. Infinite latent feature models and the indian buffet process. In Advances in neural information processing systems, pages 475–482, 2006.

[7] Peter Kairouz, H Brendan McMahan, Brendan Avent, Aur ´elien Bellet, Mehdi Bennis, Arjun Nitin Bhagoji, Keith Bonawitz, Zachary Charles, Graham Cormode, Rachel Cummings, et al. Advances and open problems in federated learning. arXiv preprint arXiv:1912.04977, 2019.

[8] Harold W Kuhn. The hungarian method for the assignment problem. Naval research logistics quarterly, 2(1-2):83–97, 1955.

[9] Mu Li, David G Andersen, Alexander J Smola, and Kai Yu. Communication efficient distributed machine learning with the parameter server. In Advances in Neural Information Processing Systems, pages 19–27, 2014.

[10] Tian Li, Anit Kumar Sahu, Manzil Zaheer, Maziar Sanjabi, Ameet
[11] Brendan McMahan, Eider Moore, Daniel Ramage, Seth Hampson, and Blaise Aguerre y Arcas. Communication-efficient learning of deep networks from decentralized data. In Artificial Intelligence and Statistics, pages 1273–1282, 2017.

[12] Mehryar Mohri, Gary Sivek, and Ananda Theertha Suresh. Agnostic federated learning. In International Conference on Machine Learning, pages 4615–4625, 2019.

[13] Adam Paszke, Sam Gross, Soumith Chintala, Gregory Chanan, Edward Yang, Zachary DeVito, Zeming Lin, Alban Desmaison, Luca Antiga, and Adam Lerer. Automatic differentiation in pytorch. 2017.

[14] Sashank J Reddi, Satyen Kale, and Sanjiv Kumar. On the convergence of adam and beyond. In International Conference on Learning Representations, 2018.

[15] Ohad Shamir, Nati Srebro, and Tong Zhang. Communication-efficient distributed optimization using an approximate newton-type method. In International conference on machine learning, pages 1000–1008, 2014.

[16] Virginia Smith, Chao-Kai Chiang, Maziar Sanjabi, and Ameet S Talwalkar. Federated multi-task learning. In Advances in Neural Information Processing Systems, pages 4424–4434, 2017.

[17] Yee Whye Teh, Dilan Gür, and Zoubin Ghahramani. Stick-breaking construction for the indian buffet process. In Artificial Intelligence and Statistics, pages 556–563, 2007.

[18] Romain Thibaux and Michael I Jordan. Hierarchical beta processes and the indian buffet process. In Artificial Intelligence and Statistics, pages 564–571, 2007.

[19] Hongyi Wang, Mikhail Yurochkin, Yuekai Sun, Dimitris Papailiopoulos, and Yasaman Khazaeni. Federated learning with matched averaging. arXiv preprint arXiv:2002.06440, 2020.

[20] Yuntao Wang, Zhou Su, Ning Zhang, and Abderrahim Benslimane. Learning in the air: Secure federated learning for uav-assisted crowdsensing. IEEE Transactions on Network Science and Engineering, 2020.

[21] Peng Xiao, Samuel Cheng, Vladimir Stankovic, and Dejan Vuko-bratovic. Averaging is probably not the optimum way of aggregating parameters in federated learning. Entropy, 22(3):314, 2020.

[22] Mikhail Yurochkin, Mayank Agarwal, Soumya Ghosh, Kristjan Greenewald, Nghia Hoang, and Yasaman Khazaeni. Bayesian non-parametric federated learning of neural networks. In International Conference on Machine Learning, pages 7252–7261, 2019.

[23] Yuchen Zhang, John C Duchi, and Martin J Wainwright. Communication-efficient algorithms for statistical optimization. The Journal of Machine Learning Research, 14(1):3321–3363, 2013.