FEDERATED MIXTURE OF EXPERTS

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ABSTRACT

Federated learning (FL) has emerged as the predominant approach for collaborative training of neural network models across multiple users, without the need to gather the data at a central location. One of the important challenges in this setting is data heterogeneity; different users have different data characteristics. For this reason, training and using a single global model might be suboptimal when considering the performance of each of the individual user's data. In this work, we tackle this problem via Federated Mixture of Experts, `FedMix`, a framework that allows us to train an ensemble of specialized models. `FedMix` adaptively selects and trains a user-specific selection of the ensemble members. We show that users with similar data characteristics select the same members and therefore share statistical strength while mitigating the effect of non-i.i.d data. Empirically, we show through an extensive experimental evaluation that `FedMix` improves performance compared to using a single global model while requiring similar or less communication costs.

1 INTRODUCTION

An ever-increasing amount of devices are being connected to the internet, sensing their environment, and generating vast amounts of data. The term federated learning (FL) has been established to describe the scenario where we aim to learn from the data generated by this "federation" of devices (McMahan et al., 2016). Not only does the number of sensing devices increase, but also their processing power is increasing continuously to the point that it becomes viable to perform inference and training of machine learning models on device. In federated learning, the goal is to learn from these client devices' data without collecting the data centrally, which naturally allows for more private exchange of information.

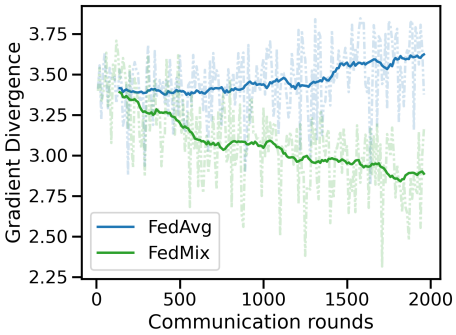


Figure 1: Gradient Divergence (defined in Appendix A), on Cifar10 in the setup of Section 4 for `FedAvg` and `FedMix` ($K = 4$).

Several challenges arise in the federated scenario. Federated devices are generally resource-constrained, both in their computational capacity as well as in communication bandwidth and latency. In a practical example, a smartphone has limited heat dissipation capacity and must communicate via Wi-Fi. From a global perspective, devices' processing power and network connection can be highly heterogeneous across geographical regions and socio-economical status of device owners, causing practical issues (Bonawitz et al., 2019) and raising questions of fairness in FL (Li et al., 2019; Mohri et al., 2019).

One of the key challenges in FL that we aim to address in this work is the non-i.i.d nature of the shards of data that are distributed across devices. In non-federated machine learning, assuming independent and identically distributed data is generally justifiable and not detrimental to model performance. In FL however, each client performs a series of parameter updates on its own data shard to amortize the costs of communication. Over time, the direction of progress across shards with non-i.i.d data starts diverging (as shown in Figure 1), which can set back training progress, significantly slow down convergence and decrease model performance (Hsu et al., 2019).

To this end, we propose Federated Mixture of Experts (`FedMix`), an algorithm for FL that allows for training an ensemble of specialized models instead of a single global model. In `FedMix`, expert

models are learning to specialize in regions of the input space such that, for a given expert, each client's progress on that expert is aligned. FedMix allows each client to learn which experts are relevant for its shard and we show how it can be extended for inference on a previously unseen client. FedMix shows competitive performance against the established standard in FL, FedAvg (McMahan et al., 2016; Deng et al., 2020) across a range of visual classification tasks. Code will be released upon publication.

2 FEDERATED MIXTURE OF EXPERTS

Federated learning (McMahan et al., 2016) deals with the problem of learning a server model with parameters $\mathbf{w}$, *e.g.*, a neural network, from a dataset $\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$ of N datapoints that is distributed across S shards, *i.e.*, $\mathcal{D} = \mathcal{D}_1 \cup \dots \cup \mathcal{D}_S$, *without* accessing the shard specific datasets directly. By defining a loss function $\mathcal{L}_s(\mathcal{D}_s; \mathbf{w})$ per shard, the total risk can be written as

$$\arg\min_{\mathbf{w}} \sum_{s=1}^{S} \frac{N_s}{N} \mathcal{L}_s(\mathcal{D}_s; \mathbf{w}), \qquad \mathcal{L}_s(\mathcal{D}_s; \mathbf{w}) := \frac{1}{N_s} \sum_{i=1}^{N_s} L(\mathcal{D}_{si}; \mathbf{w}). \tag{1}$$

It is easy to see that this objective corresponds to empirical risk minimization over the joint dataset $\mathcal{D}$ with a loss $L(\cdot)$ for each datapoint. In federated learning one is interested in reducing the communication costs; for this reason McMahan et al. (2016) propose to do multiple gradient updates for $\mathbf{w}$ in the inner optimization objective for each shard s, thus obtaining "local" models with parameters $\mathbf{w}_s$. These multiple gradient updates are denoted as "local epochs", *i.e.*, amount of passes through the entire local dataset, with an abbreviation of E. Each of the shards then communicates the local model $\mathbf{w}_s$ to the server and the server updates the global model at "round" t by averaging the parameters of the local models $\mathbf{w}^t = \sum_s \frac{N_s}{N} \mathbf{w}_s^t$. This constitutes federated averaging (FedAvg) (McMahan et al., 2016), the standard in federated learning.

One of the main challenges in federated learning is the fact that usually the data are non-i.i.d. distributed across the shards S, that is $p(\mathcal{D}|s_i) \neq p(\mathcal{D}|s_j)$ for $i \neq j$. On the one hand, this can make learning a single global model from all of the data with the classical FedAvg problematic. On the other hand, there is one extreme that does not suffer from this issue; learning S individual models, *i.e.*, only optimizing $\mathbf{w}_s$ on $\mathcal{D}_s$. Although these individual models by definition do not suffer from non-i.i.d data, clearly we should aim to do better and exchange meaningful information between clients to learn more robust and expressive models.

2.1 THE FEDMIX ALGORITHM

With FedMix, we propose to strike a balance between the two aforementioned extremes; learning a single global model and learning S individual models. For this reason, we revisit an old model formulation, the Mixture of Experts (MoE). The classical formulation of a MoE model (Jacobs et al., 1991; Jordan & Jacobs, 1994) contains a set of K experts and a gating mechanism that is responsible for choosing an expert for a given data-point. A MoE model for a data point $(\mathbf{x}, y)$ can generally be described by

$$p_{\mathbf{w}_{1:K},\theta}(y|\mathbf{x}) = \sum_{z=1}^{K} p_{\mathbf{w}_z}(y|\mathbf{x}, z) p_\theta(z|\mathbf{x}), \tag{2}$$

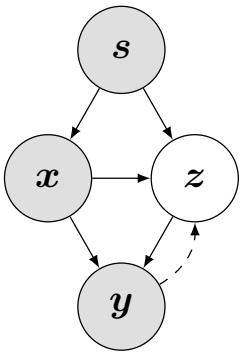


Figure 2: FedMix graphical model. The generative model is depicted with solid lines and the inference model with dashed lines.

where z is a categorical variable that denotes the expert, $\mathbf{w}_k$ are the parameters of expert k and θ are the parameters of the selection mechanism.

The MoE was proposed as a model for datasets where different subsets of the data exhibit different relationships between input $\mathbf{x}$ and output y. Instead of training a single global model to fit this relationship everywhere, each expert performs well on a different subset of the input space. The gating function models the decision boundary between input regions, assigning data-points from subsets of the input region to their respective experts.

In this work, we show that, in the federated scenario, sub-dividing the input region through a MoE can alleviate the consequences of non-i.i.d data by aligning gradient updates across experts (Figure 1). In Federated Mixture of Experts (`FedMix`) we enrich this model by conditioning the gating mechanism on the shard assignment s. Whatever characteristics make shard s different from other shards can manifest in learning a different, localized gating mechanism that does not need to be communicated to the server. In choosing $K = 1$, `FedMix` recovers the standard setting of federated averaging. $K = S$ in combination with fixing $p(z = s|\mathbf{x}, s) = 1$ recovers S independent models.

From a global perspective, we are interested in maximizing the following single objective:

$$\sum_{s}^{S}\sum_{i=1}^{N_s} \log p_{\mathbf{w}_{1:K},\theta_s}(y_{s,i}|\mathbf{x}_{s,i}, s) = \sum_{s}^{S}\sum_{i=1}^{N_s} \log \Big[\sum_{z=1}^{K} p_{\theta_s}(z|\mathbf{x}_{s,i}, s) p_{\mathbf{w}_z}(y_{s,i}|\mathbf{x}_{s,i}, z)\Big] \tag{3}$$

Given the graphical model decomposition depicted in Figure 2, the objective in Eq. 3 corresponds to a federated MoE, where we have omitted the generative models $p(x|s)$. We will briefly touch upon the role of learning generative models in Appendix C but focus on the discriminative part of the model, *i.e.*, the MoE, in this paper.

While it is possible to optimize Eq. 3 directly, we have found empirically that it is hard to achieve both: avoiding collapse to a single expert, thus obtaining `FedAvg`, and specialization of the experts. Instead, we propose to form a variational lower-bound on Eq. 3 with a global variational approximation $q_\phi(z|\dots)$ to the true posterior $p(z|\mathbf{x}, y, s)$ with parameters $\boldsymbol{\phi}$. At test time, $p(y|\mathbf{x}^*, s) = \sum_{k=1}^{K} p(y|\mathbf{x}^*, z)p(z|\mathbf{x}^*, s)$ can be readily evaluated without requiring q. This allows us to condition $q_\phi(z|\dots)$ on any available side-information *at training time* that might result in better specialization in the non-i.i.d federated scenario. In this paper we mainly consider classification tasks whose non-i.i.d nature predominantly stems from the non-i.i.d distribution of labels y. Other or additional known sources of misalignment could be included to further improve this approximation, such as a manufacturer-id for a medical device in a medical scenario, a geographic identifier, or general domain-specific information. We show one such additional example in 4.2. The lower bound to be maximized in `FedMix` therefore is as follows:

$$\sum_{s}^{S}\sum_{i=1}^{N_s} \log p_{\mathbf{w}_{1:K},\theta_s}(y_{s,i}|\mathbf{x}_{s,i}, s) \tag{4}$$

$$\geq \sum_{s}^{S}\sum_{i=1}^{N_s}\sum_{z=1}^{K} q_\phi(z|y_{s,i})[\log p_{\mathbf{w}_z}(y_{s,i}|\mathbf{x}_{s,i}, z)p_{\theta_s}(z|\mathbf{x}_{s,i}, s) - \log q_\phi(z|y_{s,i})] \tag{5}$$

$$= \sum_{s}^{S}\sum_{i=1}^{N_s}\left(\sum_{z=1}^{K} q_\phi(z|y_{s,i})[\log p_{\mathbf{w}_z}(y_{s,i}|\mathbf{x}_{s,i}, z)p_{\theta_s}(z|\mathbf{x}_{s,i}, s)]\right) + H(q_\phi(z|y_{s,i})). \tag{6}$$

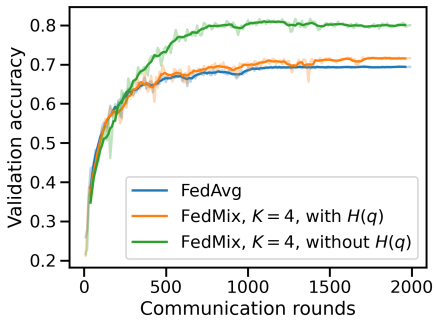


Figure 3: The effect of specialisation (without $H(q)$) compared to an ensemble (with $H(q)$) and `FedAvg`. The experimental setup is identical to what is described in Section 4.

Conditioning only on y allows us to efficiently parameterize the variational approximation, incurring only a small communication overhead. While it would be possible to condition $q_\phi(z|y)$ on s, thus having localized approximations with parameters ϕ_s that do not need to be communicated, we found a global approximation to help align the gating mechanisms across shards. A global $q_\phi(z|y)$ encourages shards that contain data with the same label to assign them to the same expert.

Specialization of the experts is a key ingredient for `FedMix` to be successful; with specialization, the gradients for each expert become aligned across shards (see Figure 1), the hold-out accuracy improves (see Figure 3), and the communication costs decrease as each shard may only need to access a subset of the experts. We find that performing maximum a-posteriori (MAP) inference for z generally leads to better and more personalized models. By removing the entropy term from equation 4, $q_\phi(z|y)$ and therefore $p_{\theta_s}(z|\mathbf{x}, s)$ are encouraged to concentrate and select only one expert for a

given data point. In the extreme case where a client's shard contains only data that is assigned to the same expert, we can reduce communication by receiving and sending updates for that single expert only. We show in Section 4 that communicating and evaluating experts based on thresholding the aggregate $q_\phi(z|s) = \mathbb{E}_{y\sim D_s}[q_\phi(z|y)]$ can reduce communication and computation overhead.

Figure 3 compares `FedMix` with and without the entropy term to standard `FedAvg` as a function of communication steps. With the entropy term, `FedMix` develops no expert specialization and collapses to an ensemble of $K = 4$ models. One drawback of the heavy specialization with MAP inference is that sometimes `FedMix` prematurely completely prunes experts, *i.e.*, $p_{\theta_s}(z = k|\mathbf{x}, s) \approx 0 \;\; \forall \mathbf{x}, s$. This can be undesirable as we lose model capacity that can be used for better modeling the data. As $q_\phi(z|y)$ is one of the main training signals of $p_{\theta_s}(z|\mathbf{x}, s)$, we introduce the marginal entropy term in the server, $H(E_{p(y)}[q_\phi(z|y)])$, as a regularizer. Notice that this leads to different training dynamics than locally optimizing the lower bound with the entropy included and we, empirically, found that it alleviates premature pruning, while still leading to specialized models. Figure 9 in Appendix D visualizes the development of $q_\phi(z|y)$ over time from initially uniform to high specialisation for the experiment depicted in Figure 3.

Server Side Updates In a general federated learning algorithm, a central server selects a subset $S' \subset \{1, \dots, S\}$ of clients at time t and transmits the current estimate of the global parameters $\mathbf{w}^t$ to them. These clients perform a series of mini-batch gradient updates with data from their shard $\mathcal{D}_s$ on a local loss function, which can come at the price of each client moving in possibly different directions in parameter space. In generalized `FedAvg` (Reddi et al., 2020), the server interprets $\Delta_s^t = \mathbf{w}^t - \mathbf{w}_s^{t+1}$ as a single-step gradient update from client s, averages those gradients and applies an optimizer such as Adam (Kingma & Ba, 2014) to receive $\mathbf{w}^{t+1}$. In light of non-i.i.d data across clients, this averaging strategy can result in slow progress since averaging updates in a highly non-convex parameter space can be sub-optimal. In `FedMix`, this effect is mitigated since for a given expert, the data that is used to update its parameters are aligned better across shards.

`FedMix` offers a second way to improve convergence speed by modifying the server-side updates. In generalized `FedAvg`, the individual gradients returned by the subset S' of clients are averaged according to

$$\Delta^t = \sum_{s=1}^{S'} p(s) \cdot \Delta_s^t \,, \quad p(s) = \frac{N_s}{N_{S'}}. \tag{7}$$

In `FedMix`, we can speed up convergence by considering expert-specific updates $\Delta_{k,s}^t = \mathbf{w}_k^t - \mathbf{w}_{k,s}^{t+1}$. If a client s pruned away expert k from its local gating mechanism, $\Delta_{k,s}^t$ will be zero. We propose to normalize the effective magnitude of the resulting update Δ_k by up-weighing the updates of all other clients that do consider expert k for their local mixture:

$$\Delta_k^t = \sum_{s=1}^{S'} p(s|z = k) \cdot \Delta_{k,s}^t \,, \quad p(s|z = k) \propto p(z = k|s)p(s) \,, \quad p(s) = \frac{N_s}{N_{S'}}. \tag{8}$$

Computing $p(z|s) = \mathbb{E}_{\mathbf{x}\sim\mathcal{D}_s}[p_{\theta_s}(z|s, \mathbf{x})]$ prior to sending updates to the server involves evaluating potentially large neural network models. Therefore we choose to approximate $p(z|s) \approx q_\phi(z|s) = \mathbb{E}_{y\sim\mathcal{D}_s}[q_\phi(z|y)]$, which involves just a single matrix multiplication.

Pruning experts Maintaining the cheap-to-compute marginal posterior per shard offers an additional opportunity to increase computation speed during local shard iterations and reduce overall communication costs. We propose to "prune away" experts locally from the MoE if $q_\phi(z|s)$ does not surpass a threshold η/K. In order to still optimize a valid bound, we need to re-normalize $q_\phi(z|y)$ before evaluation of the loss function (Pal et al., 2005). We evaluate the same threshold prior to sending updates to the server in order to avoid communicating parameters that have not changed during the client's iterations. Once the server selects a client for another round, it provides only those experts to the client that were updated by the client in the previous round. We empirically find that the entropy of $q(z|s)$ decreases steadily and we prune away experts k with probability $q(z = k|s) < \eta/K$ without significant drop in performance. We explore the consequences of pruning experts in the experiment section and in Appendix B. Algorithm 2 shows how `FedMix` can be enriched by pruning.

Algorithm 1 The `FedMix` algorithm. α, β are the client and server learning rates respectively

function SERVER SIDE
  Initialize $\boldsymbol{\phi}$ and K vectors $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_K]$
  for round t in $1, \dots T$ **do**
    $S' \leftarrow$ random subset of the clients
    Initialize $\Delta^t_{\mathbf{W}} = \mathbf{0}, \Delta^t_{\boldsymbol{\phi}} = \mathbf{0}$
    for s in S' **do**
      $\mathbf{W}^t_s, \boldsymbol{\phi}^t_s, p(z|s) \leftarrow$ CLIENT SIDE$(s, \boldsymbol{\phi}, \mathbf{W})$
    end for
    $p(s|z) \leftarrow p(z|s)p(s) / \sum_{s \in S'} p(z|s)p(s)$
    for s in S' **do**
      $\Delta^t_{\mathbf{w}_k} += p(s|z=k)(\mathbf{w}^{t-1}_k - \mathbf{w}^t_{s,k}) \;\; \forall k$
      $\Delta^t_{\boldsymbol{\phi}} += \frac{N_s}{N_{S'}}(\boldsymbol{\phi}^{t-1} - \boldsymbol{\phi}^t_s)$
    end for
    $\Delta^t_{\boldsymbol{\phi}} -= \nabla_{\boldsymbol{\phi}} H(\sum_c q_\phi(z|y=c)p(y=c))$
    $\mathbf{w}^{t+1}_{1:K} \leftarrow$ ADAM$(\Delta^t_{\mathbf{w}_{1:K}}, \beta)$
    $\boldsymbol{\phi}^{t+1} \leftarrow$ ADAM$(\Delta^t_{\boldsymbol{\phi}}, \beta)$
  end for
end function

function CLIENT SIDE$(s, \boldsymbol{\phi}, \mathbf{W})$
  Get local parameters θ_s
  for epoch e in $1, \dots, E$ **do**
    for batch $b \in B$ **do**
      $L_s \leftarrow \mathbb{E}_{q_\phi(z|y_b)}[\log p_{\mathbf{w}_z}(y_b|\mathbf{x}_b, z) p_{\theta_s}(z|\mathbf{x}_b, s)]$
      $\boldsymbol{\phi} += \alpha \nabla_{\boldsymbol{\phi}} L_s$
      $\mathbf{W} += \alpha \nabla_{\mathbf{W}} L_s$
      $\theta_s += \alpha \nabla_{\theta_s} L_s$
    end for
  end for
  $q(z|s) \leftarrow \mathbb{E}_{y \sim \mathcal{D}_s}[q_\phi(z|y)]$
  return $\mathbf{w}_{1:K}, \boldsymbol{\phi}, q(z|s)$
end function

Designing robust gates In the federated scenario, N_s is often much smaller than N and especially small in relation to the complexity of the data we try to model. Any localized parameters therefore are prone to overfitting. On the other hand, the global parameters of an expert are trained using all data-points assigned to that expert across all shards, allowing to learn more robust features.

We can make use of the robustness of these experts' features for the gating mechanism by conditioning on them instead of training an entirely separate model for $p_{\theta_s}(z|\mathbf{x}, s)$. Let us define $h_k(\mathbf{x})$ as intermediary features of expert k. Since not all experts might be used for a given shard and in order to scale with K, we average over the marginal posterior of the training set at that shard before applying a linear transformation to compute the input to the softmax gates:

$$h_s(\mathbf{x}) = \sum_{k=1}^{K} q_\phi(z=k|s) h_k(\mathbf{x})$$

$$p_{\theta_s}(z|\mathbf{x}, s) = \text{SM}\left(\mathbf{A}_s^T h_s(\mathbf{x}) + \mathbf{b}_s\right) \tag{9}$$

where $\theta_s = (\mathbf{A}_s, \mathbf{b}_s)$ are local learnable parameters and SM represents the softmax function.

Inference at test time We consider three variants for test-time evaluation of `FedMix`. In the first case, a client s that participated in training is presented with a new data point $(\mathbf{x}^*, s)$. Predictions can then be straightforwardly done by selecting the y that maximizes $\sum_{z=1}^{K} p(y|\mathbf{x}^*, z) p(z|\mathbf{x}^*, s)$. In the second, more challenging, scenario a new client s^* is introduced together with a new labelled local data set $\mathcal{D}_{s^*}$. Here we propose to instantiate and train the local gating mechanism by optimizing the parameters θ_s of $p_{\theta_s}(z|\mathbf{x}, s^*)$ via MAP inference at the local objective. Afterwards, predictions can be made in a manner similar to the first case.

Finally, we consider the case in which a new client s^* has no labelled dataset available. Without a local gating function, simply ensembling experts exhibits almost random behaviour since experts can be overly confident on out-of-distribution data (Snoek et al., 2019). We therefore propose to ensemble across local gating mechanisms to compute $p(z|\mathbf{x}^*) = \sum_{s=1}^{S} p_{\theta_s}(z|\mathbf{x}^*, s) p(s|\mathbf{x}^*)$; a method which works well in practice. In Appendix C we discuss results for new shard inference as well as a more principled approach which makes use of the graphical model formulation in Figure 2.

3 RELATED WORK

`FedMix` has similarities to many recent works in the topic of federated learning. Two methods closely related to ours are described in (Sattler et al., 2019; Briggs et al., 2020). The authors propose to perform hierarchical clustering on the updates returned from each shard in order to incrementally create separate models for groups of users, with a cluster assignment mechanism based on hand-crafted heuristics. `FedMix` instead takes a different approach; it starts with a fixed set of K models

and then optimizes with gradient descent at each shard a per-datapoint model assignment mechanism that can better fit the peculiarities of the local dataset.

Another closely related work is presented by Mansour et al. (2020), where the authors propose to similarly create an ensemble of K-models and assign to each shard the model that achieves the lowest training loss on the local dataset. This is closer to the assignment that happens in `FedMix` with one main difference; `FedMix` takes into account the uncertainty in the selection mechanism as well with $p(z|\mathbf{x}, s)$ instead of selecting the top performing component during training. This is beneficial early in training where the models have not fully specialized yet. Using local and global model parts has also been explored by Liang et al. (2020). The authors propose to have a local feature extractor at each shard and a global classifier on top of those features as opposed to having K-separate models and a local selection mechanism as in `FedMix`. This setup yields improvements upon the vanilla federated averaging algorithm, however there are two potential drawbacks; first, empirically, the authors had to start their procedure from a pre-trained model with `FedAvg` and secondly, they have to ensemble all of the different feature extractors for predictions in new shards. In our experiments, we omit the pre-training step and show that the ensembling strategy fails.

Federated learning in the non-i.i.d setting can also be improved upon in other ways. Li et al. (2018) propose to employ a proximal regularizer at the shard level in order to prevent the local models from drifting too far from the global model, thus making federated learning more robust. Jiang et al. (2019) notice that `FedAvg` and Reptile (Nichol et al., 2018), a meta-learning algorithm, are essentially the same algorithm and thus propose fine tuning with Reptile in order to improve the personalized performance of the global model. In a similar vein, there are promising new works that explore the meta-learning view of federated learning (Chen et al., 2018; Khodak et al., 2019; Fallah et al., 2020). Improving the personalized performance of the global model has also been done without meta-learning in works such as by Deng et al. (2020); Mansour et al. (2020). In general, such improvements are complementary to `FedMix` and can be used to further enhance its performance. We refer the interested readers to the recent surveys by (Kairouz et al., 2019; Kulkarni et al., 2020).

4 EXPERIMENTS

We evaluate `FedMix` on three datasets: Cifar10, Cifar100 (Krizhevsky et al., 2009) and Femnist (Caldas et al., 2018), a 62-way image classification problem on hand-written digits and letters that is naturally non-i.i.d due to different writing styles of 3500 users. In Appendix B we provide additional ablation studies.

For Cifar10, we replicate the federated data split of Hsu et al. (2019). The dataset is split across 100 clients, whose data-points are drawn according to their label from a Dir$(\alpha = 1.0)$ distribution without replacement. For the base model, we use a LeNet-5 architecture (LeCun et al., 1998). We use a SGD optimizer with a learning rate of 0.05 and a batch size $B = 64$ locally and the Adam (Kingma & Ba, 2014) optimizer with its default hyperparameters at the server by interpreting the difference of the local from the global model as a gradient (Reddi et al., 2020). We sample 10 clients without replacement on each round (but with replacement across rounds) and train for $E = 1$ local epochs. For Cifar100 we replicate the data split of Reddi et al. (2020). The dataset is split into 500 clients by using a hierarchical model over the coarse and fine labels, with the same hyperparameters as the ones provided by Reddi et al. (2020). The other hyperparameters are the same as Cifar10 with the exception of the batch size, where we use $B = 20$, as well as the architecture, where we use a ResNet-20 with group normalization (Wu & He, 2018) layers instead of batch normalization (Ioffe & Szegedy, 2015). We augment the data by random cropping from a 4 pixel padded image and horizontal flipping. Finally, for the Femnist dataset[1] , we similarly followed the setup of Reddi et al. (2020) with the same LeNet-5 architecture and hyperparameters of Cifar10 with the exception of the batch size where we used $B = 20$. For Cifar10 and Cifar100, $h_k(\mathbf{x})$ is defined as the input to an expert's output layer. For Femnist, we observed significant overfitting with the same definition, so we set $h_k(\mathbf{x})$ to be the output logits for each expert.

[1]At the time of submission, the Local/Global (Liang et al., 2020) experiments have not finished so we can not report their results. Initially, they have similar evolution to `FedAvg`.

4.1 PERFORMANCE VS. COMMUNICATION

We compare FedMix along several dimensions to baselines such as (generalized) FedAvg (Reddi et al., 2020), *biased* FedAvg, and the Local/Global approach of Liang et al. (2020). In *biased* FedAvg, we allow each client to learn a personalized bias vector b_s of its output layer. This will allow *biased* FedAvg to model the label skew at each client but, fundamentally, cannot model any other form of non-i.i.d-ness. Similarly, Liang et al. (2020) propose to split the model into local and global components by having local feature extractors and learning the upper layers of the neural network via FedAvg. We experimented with splitting LeNet-5 at every intermediate layer and report results with the best performing split: keeping the input layer local. For ResNet-20, splitting after the first block performed best. First, we show that training with FedMix achieves higher global model accuracy. Second, we show that for a given communication budget, FedMix can be competitive against baselines. Table 1 contains test set results for Cifar10, evaluated after $2k$ communication steps and Femnist evaluated after $5.95k$. Figures 4d, 4f reveal that the models have converged at that point. For Cifar100, we observe no overfitting and report test-set accuracies averaged over the last 10 evaluations. Figure 4 shows learning curves for different settings of FedMix.

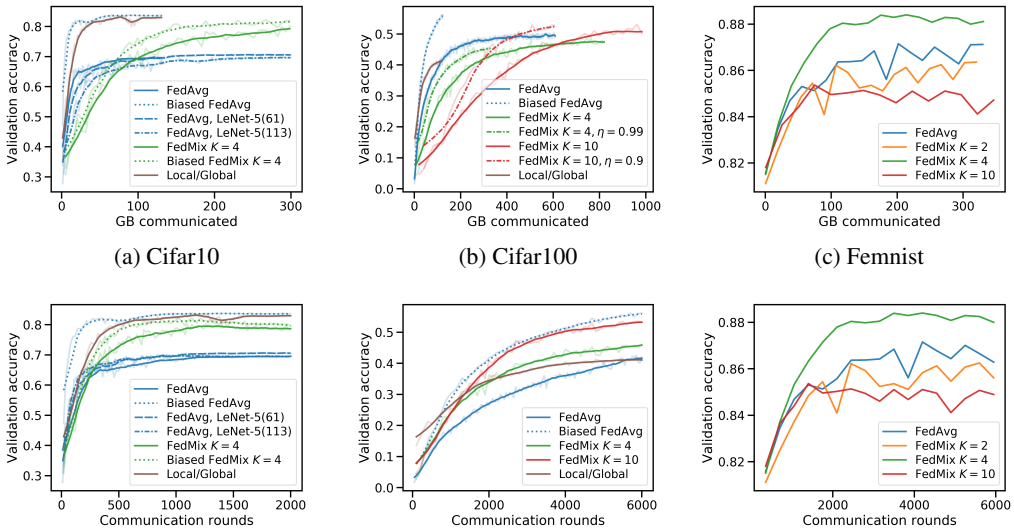
For **Cifar10** we can see that except for the initial training phase, FedMix improves over FedAvg for a given communication budget. For the same communication costs per communication round, FedMix offers better performance than FedAvg, as can be seen in comparing FedMix ($K = 2$) to FedAvg LeNet-5 with 61 channels and FedMix ($K = 4$) to FedAvg LeNet-5 with 113 channels. The channel count has been chosen such that the model size approximates 2 and 4 separate standard LeNet experts respectively. Against *biased* FedAvg and Local/Global Liang et al. (2020), FedMix can improve significantly in terms of inference on a new shard (Figure 8 in Appendix C). When endowing FedMix with the ability to learn a single personalized bias vector b_s across all experts, we can harness some of the advantages of *biased* FedAvg for inference on a new shard while retaining FedMix' advantage when performing inference on a new shard.

For **Cifar100**, we can see that learning progresses much faster for FedMix in terms of communication rounds than FedAvg. Against FedAvg, we can see that FedMix improves with both K=4 and K=10 on a per round progression, and with K=10 and expert pruning, it eventually provides a better accuracy and communication trade-off than FedAvg. *Biased* FedAvg seems to be the better inductive bias in this task, although one should be weary that its usefulness is limited to label skew and does not generalize to other sources of non-i.i.d.ness (see section 4.2). This is in contrast to FedMix which is designed to handle any type of explicit non-i.i.d.ness.

For **Femnist** we compare against FedAvg and observe that generally FedMix is more prone to overfitting due to the extra amount of model parameters and expert specialization. For this reason, we tie the parameters of all the layers of the LeNet-5 experts, except for those at the output layer. In this setting, the extra communication cost of FedMix compared to FedAvg is negligible and with $K = 4$ experts we see that FedMix reaches better performance. Alternative choices for K, such as $2, 10$, did not seem to improve upon FedAvg or $K = 4$. *Biased* FedAvg performed identically to standard FedAvg since the non-i.i.d-ness does not predominantly stem from label-skew.

Table 1: Average test-set accuracies across clients and communication costs (rounds and GB) for Cifar10, Cifar100 and Femnist. For Cifar10 we report the performance after $2k$ rounds, for Cifar100 we report the average over the last 10 evaluations at the end of training and for Femnist we report after $5.95k$ communication rounds.

Method	Cifar 10		Cifar 100		Femnist	
	Acc.	Comm.	Acc.	Comm.	Acc.	Comm.
FedAvg	69.36%	$2k, 137.3GB$	49.58%	$30k, 608GB$	86.29%	$5.95k, 282.4GB$
biased FedAvg	83.9%	$2k, 130.92GB$	56.14%	$6k, 123.1GB$		
Liang et al. (2020)	83.16%	$2k, 129.93GB$	41.09%	$6k, 116.7GB$		
FedMix K=2	72.25%	$2k, 261.4GB$	48.29%	$30k, 1130GB$	85.61%	$5.95k, 283.4GB$
FedMix K=4	79.88%	$2k, 522.5GB$	48.55%	$24k, 1972GB$	88.00%	$5.95k, 312.3GB$
FedMix K=10	80.00%	$2k, 1304.1GB$	52.59%	$6k, 1130GB$	84.89%	$5.95k, 399.0GB$



(a) Cifar10 (b) Cifar100 (c) Femnist

(d) Cifar10 (e) Cifar100 (f) Femnist

Figure 4: Average accuracy across all clients (y-axis) as a function of the amount of GB communicated (top row) and as a function of communication rounds (bottom row). Cifar 10 models are trained on the standard 45k training split. x-axes have been truncated for improved visibility. Best viewed in color.

4.2 Rotated MNIST

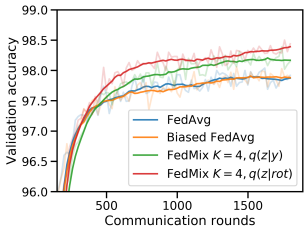


Figure 5: Only rotation

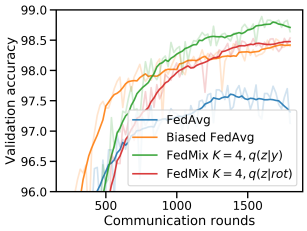


Figure 6: Rotation and labels

To show that `FedMix` is not limited to label-skew, we create a federated rotated MNIST dataset with 100 clients. Instead of label skew, each client randomly chooses a multiple of 45 degrees from a different probability distribution over 8 possible rotation angles to rotate a digit with. Each client's distribution is drawn from Dir($\alpha = 1.0$). At test time, each data-point is randomly rotated according to the client's distribution. Additionally, we create a dataset where instead of uniform sampling of labels, we replicate the non-i.i.d label skew described for Cifar10 above and combine it with the rotation non-i.i.d-ness. We compare `FedMix` where q is conditioned on y or on the degrees of rotation for a data-point against baselines. Figures 5 and 6 show that *biased* `FedAvg` can improve in the presence of label skew but collapses to standard `FedAvg` for rotation non-i.i.d-ness. `FedMix` on the other hand has an advantage in both cases. Furthermore, in presence of both sources of non-i.i.d-ness, `FedMix` with $q(z|y)$ can outperform *biased* `FedAvg`. In the presence of only rotation (Figure 5), conditioning `FedMix` on the true source of non-i.i.d-ness is advantageous.

5 Discussion

With `FedMix` we have introduced a federated learning algorithm that explicitly takes the non-i.i.d characteristics of a federated dataset into account. Clients can learn to align specialized experts on sub-regions of the data space and achieve higher performance compared to `FedAvg`, especially in situations where the source of the non-i.i.d nature is known. This assumption is very strong in real-world federated scenarios and we expect a more flexible alignment process than a global $q(z|y)$ to be the most interesting avenue for future research. Nevertheless, we do show some encouraging results on the rotated MNIST experiment, where even with the "wrong" conditioning we were able to improve upon `FedAvg`. In the future, we will explore ways to perform automatic selection of K as well as automatic selection of architecture elements to share between experts, trading-off gradient alignment and communication budgets.

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A GRADIENT DIVERGENCE

We aim to track the divergence of updates for a subset S' of shards at the server at time step t for `FedMix` and `FedAvg`. Therefore we define a metric inspired by Kim et al. (2020); Sattler et al. (2019) to define divergence of gradients $\Delta^t_{k,i} = \boldsymbol{\omega}^t_k - \boldsymbol{\omega}^{t+1}_{k,i}$ for some subset $\boldsymbol{\omega}_k$ of the parameters $\mathbf{w}_k$ of expert k as

$$\text{GD}(\Delta^t_k) = \sum_{i=1}^{S'} \sum_{j=1}^{S'} p(s=i|z=k)p(s=j|z=k) \cdot 0.5 \cdot \left(1 - \frac{\Delta^t_{k,i} \cdot \Delta^t_{k,j}}{||\Delta^t_{k,j}|| \cdot ||\Delta^t_{k,i}||}\right). \tag{10}$$

For `FedAvg`, the above metric collapses to

$$\text{GD}(\Delta^t) = \sum_{i=1}^{S'} \sum_{j=1}^{S'} p(s=i)p(s=j) \cdot 0.5 \cdot \left(1 - \frac{\Delta^t_{i} \cdot \Delta^t_{j}}{||\Delta^t_{j}|| \cdot ||\Delta^t_{i}||}\right). \tag{11}$$

In Figure 1 in the main text, we plot the sum of $\text{GD}(\Delta^t_k)$ across all parameters $\boldsymbol{\omega}_k$ (*i.e.*, convolutional kernels, weights and biases) of the LeNet-5 experts in comparison to $\boldsymbol{\omega}$ for `FedAvg`.

B ABLATION STUDIES

We investigate the characteristics of `FedMix` by varying the number of experts K for Cifar10, as well as by selecting different levels η for pruning experts. Figures 7a and 7c show learning curves of several values of K. We can see that a higher number of experts has the potential to achieve higher accuracies at the cost of more required communication. With increasing K, the modeling task for a single expert becomes progressively easier and the challenge is moved towards identifying the right expert for a given data-point. This could subsequently lead to overfitting in the federated setting if not for the shared feature extractor $h(\mathbf{x})$ (Eq. equation 9). In case we choose K to be equal to the number of classes, we observe that `FedMix` assigns one cluster to each class and the $p(z|\mathbf{x}, s)$ is reminiscent of Liang et al. (2020). In case we further increase K, we observe marginally improved performance by multiple experts being assigned to the same label.

Figures 7b and 7d depict the influence of different pruning levels η on the communication efficiency and final performance `FedMix` with $K = 4$. We can see that higher levels of pruning do reduce communication significantly, however they cause some loss of performance.

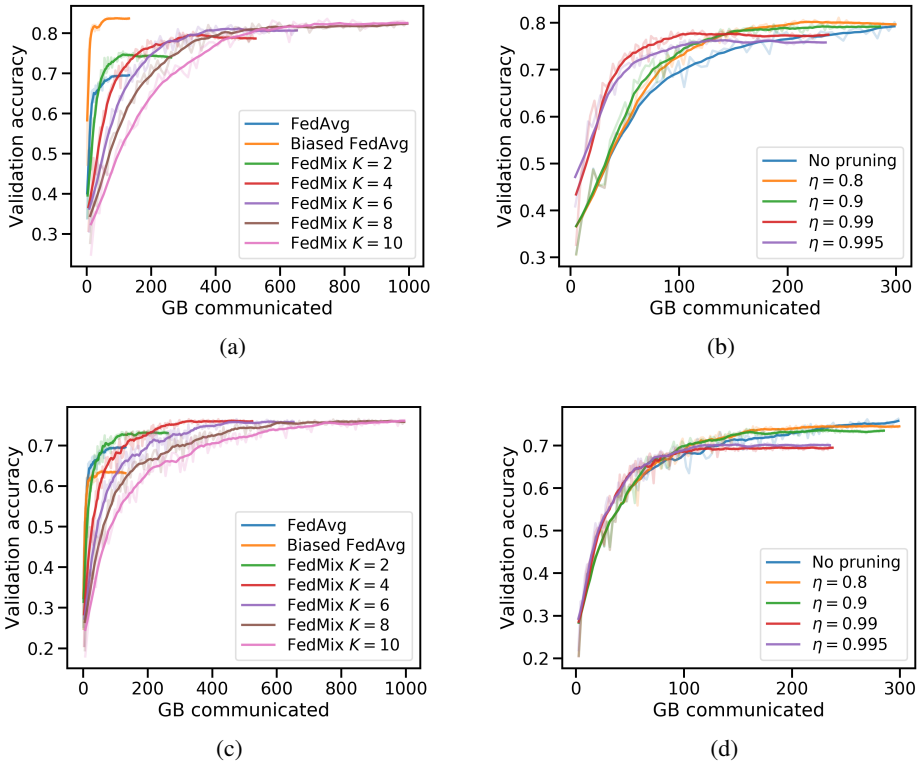
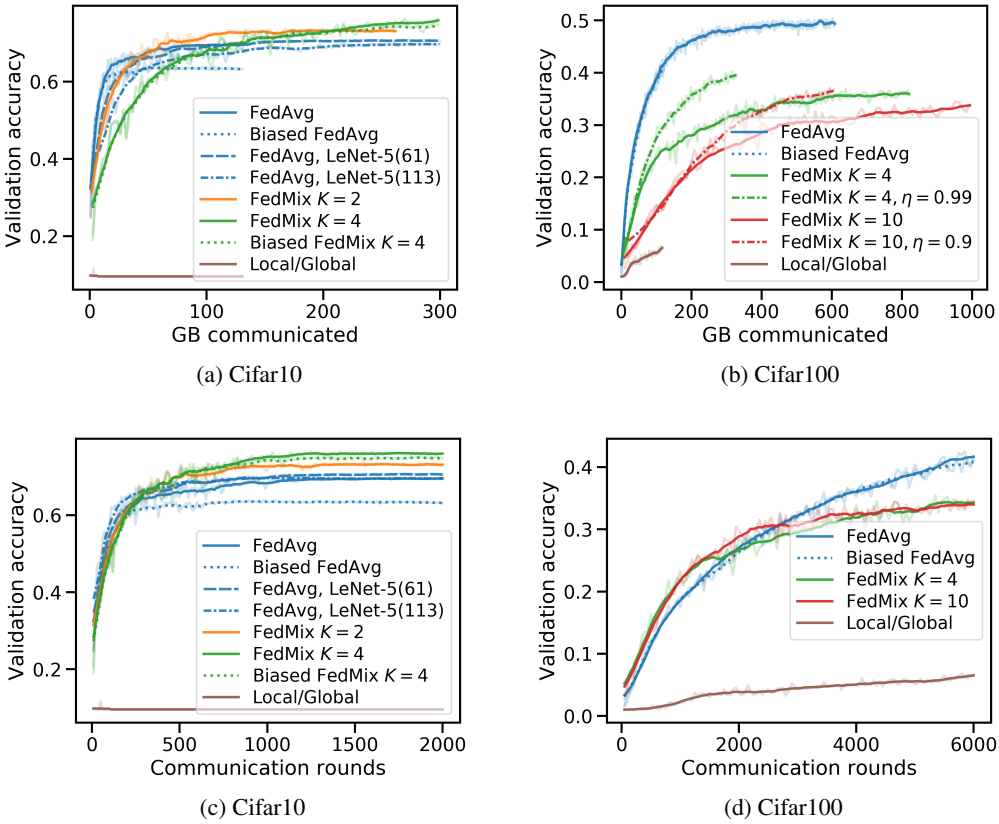


Figure 7: Ablation studies on the effect of K on the average local accuracy (**a**) and new shard accuracy (**c**) as well as on the influence on local (**b**) and new shard (**d**) accuracy of the threshold for pruning experts before communication for $K = 4$

C New shard inference

In the main text, we discussed performance of the individual algorithms when evaluating new data on a shard that took part in training and therefore has access to trained local model parameters. This is the case for all considered methods except `FedAvg`, for which there exist no localized parameters. For inference on a new shard, we use the sum of all local validation sets as a proxy. Liang et al. (2020) propose to ensemble the representations of the local feature extractors across clients before evaluating the global part of the network. We find this approach to work quite poorly in practice. Presumably pretraining the local feature extractors with `FedAvg` ameliorates this behaviour. In *biased* `FedAvg`, we ensemble the individual local biases across clients to receive a single global bias. For `FedMix`, we marginalize the local gating predictions to achieve a global gating prediction $p(z|\mathbf{x}^*) = \sum_{s=1}^{S} p_{\theta_s}(z|\mathbf{x}^*, s)p(s)$. Predictions can then be made by marginalizing across experts using this global gating function: $p(y|\mathbf{x}^*) = \sum_{z=1}^{K} p_{\mathbf{w}_k}(y|\mathbf{x}^*, z)p(z|\mathbf{x}^*)$.

Interestingly, Cifar10 and Cifar100 display different behaviours when comparing `FedMix` to the baselines. For Cifar10, *biased* `FedAvg` performs much worse compared to `FedAvg` while `FedMix` performs well. For Cifar100, *biased* `FedAvg` is indistinguishable from `FedAvg`, outperforming `FedMix`. We leave the investigation of these discrepeancies to future work.



(a) Cifar10 (b) Cifar100

(c) Cifar10 (d) Cifar100

Figure 8: Accuracy on a new client (y-axis) as a function of the amount of GB communicated (top row) and as a function of communication rounds (bottom row). Cifar 10 models are trained on the standard 45k training split. x-axes have been truncated for improved visibility. Best viewed in color.

As an alternative to marginalizing the local gate predictions using $p(s)$, investigating the graphical model in Figure 2 reveals the possibility for marginalization with $p(s|\mathbf{x}^*)$:

$$p(z|\mathbf{x}^*) = \sum_{s=1}^{S} p_{\theta_s}(z|\mathbf{x}^*, s)p(s|\mathbf{x}^*), \quad p(s|\mathbf{x}^*) \propto p(\mathbf{x}^*|s)p(s). \tag{12}$$

It is for this third evaluation case that training local generative models $p(\mathbf{x}|s)$ for each client becomes interesting, as they allow to compute the responsibilities $p(s|\mathbf{x}^*)$ at test time. In practice, however, the success of this approach depends heavily on the correctness of $p(s|\mathbf{x}^*)$, which in turn depends on the ability of the local generative models $p(\mathbf{x}|s)$ to assign high probability to data that resembles $\mathcal{D}_s$ and low probability to out-of-distribution data. Training and calibrating generative models for this task is in itself an active area of research (Nalisnick et al., 2018) and investigating how clients in a federated setting might exchange information to facilitate this process is not yet explored. We therefore leave a thorough evaluation of this case to future work and only present here a MNIST (LeCun et al., 2010) experiment.

We train `FedMix` with $K = 4$ and experts of two hidden layer ReLU MLP with 200 hidden units on MNIST. We split the dataset into $S = 100$ clients according to the procedure described in Liang et al. (2020). `FedMix` achieves 97.7% average validation accuracy compared to 97.0% with `FedAvg` after 600 communication steps. Independently for each client, we train a small variational autoencoder with a 32-dimensional latent space using a two-layer MLP with 512 and 256 hidden units respectively as encoder and mirrored decoder structure. We optimize the VAEs using Adam with standard hyper parameters, $B = 10$ and perform early stopping on the local validation sets after no improvement for three epochs. After training, each client communicates their VAE

to the server, where we evaluate $p(s|\mathbf{x}^*)$ to marginalize over the local gating functions according to $p(z|\mathbf{x}^*) = \sum_{s=1}^{S} p(z|\mathbf{x}^*, s)p(s|\mathbf{x}^*)$. With this procedure, FedMix achieves 95.9% test set accuracy, compared to FedAvg with 96.9%. Marginalizing with $p(s)$ instead of $p(s|\mathbf{x}^*)$ achieves 96.63%, showing the limitation of the approach in that any error in $p(s|\mathbf{x}^*)$ propagates into the expert assignment. Reliable out-of-distribution detection capabilities in the individual estimators for $p(\mathbf{x}|s)$ are therefore necessary.

D SPECIALIZATION

In Figure 9 we see how $q_\phi(z|y)$ changes over time. The entropy of $q_\phi(z|y = c)$, i.e. the weight with which each expert is assigned to a specific label c decreases over time until each label is assigned exactly one expert with probability 1.

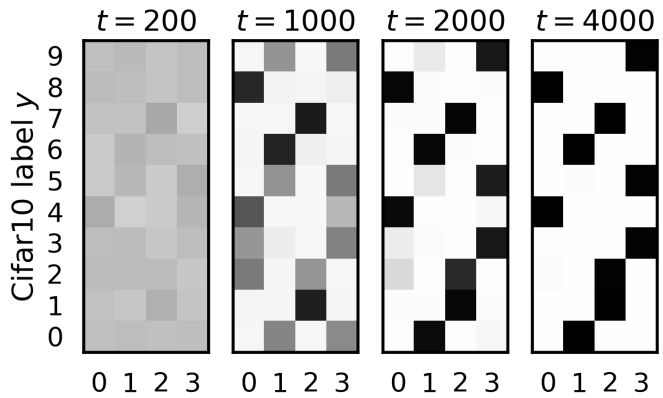


Figure 9: Visualization of $q_\phi(z|y)$ at different communication rounds t for FedMix with $K = 4$ on Cifar10. Greyscale corresponds to probabilities; white corresponds to zero and black corresponds to one. Probabilities sum to one across experts (horizontally).

E FEDMIX WITH EXPERT PRUNING

The FedMix algorithm (Algorithm 1) can be extended to ignore the communication of experts between server and client if, for this given client, that particular expert is not updated during training. If $q_\phi(z = k|s) = E_{p(y|s)}[q_\phi(z = k|y)] = 0$ for an expert k on client s, then parameters of that expert observe no gradient and the expert is effectively pruned from the local library of available experts. Since the parameterization of $q_\phi(z|s)$ does not allow for exact values of zero, we introduce η, such that if $q_\phi(z = k|s) < \eta/K$, we consider expert k to be pruned. Since the value of $q_\phi(z = k|s)$ during local optimization at the client is subject to change, it is possible that $q_\phi(z = k|s)$ briefly lies above the threshold even though it had just been pruned away. Therefore the server considers expert k pruned for a given client s' only if $q_\phi(z = k|s = s') < 0.9 \cdot \eta/K$. Algorithm 2 details this approach. Note that we write $p(z|s) = \mathbb{E}_{\mathbf{x}\sim D_s}[p_{\theta_s}(z|\mathbf{x}, s)]$, i.e. the true marginal, however in practice we make use of the cheap to compute marginal approximation $q_\phi(z|s) = \mathbb{E}_{y\sim D_s}[q_\phi(z|y)]$.

Algorithm 2 The `FedMix` algorithm. α, β are the client and server learning rates respectively, $\eta \in [0, 1]$ is the pruning threshold

function SERVER SIDE
  Initialize $\boldsymbol{\phi}$ and K vectors $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_K]$
  for round t in $1, \ldots T$ **do**
    $S' \leftarrow$ random subset of the clients
    Initialize $\Delta^t_{\mathbf{W}} = \mathbf{0}, \Delta^t_{\boldsymbol{\phi}} = \mathbf{0}$
    Initialize $p(z|s) = 1/K \forall s$
    for s in S' **do**
      $\mathbf{W}' \leftarrow [\mathbf{w}_k \,|\, p(z = k|s) \geq 0.9 \cdot \eta/K]$
      $\mathbf{W}^t_s, \boldsymbol{\phi}^t_s, p(z|s) \leftarrow$ CLIENT SIDE$(s, \boldsymbol{\phi}, \mathbf{W}')$
      Store $p(z|s)$
    end for
    $p(s|z) \leftarrow p(z|s)p(s)/\sum_{s \in S'} p(z|s)p(s)$

    for s in S' **do**
      $\Delta^t_{\mathbf{w}_k} += p(s|z = k)(\mathbf{w}^{t-1}_k - \mathbf{w}^t_{s,k}) \;\; \forall k$
      $\Delta^t_{\boldsymbol{\phi}} += \frac{N_s}{N_{S'}}(\boldsymbol{\phi}^{t-1} - \boldsymbol{\phi}^t_s)$
    end for
    $\Delta^t_{\boldsymbol{\phi}} -= \nabla_{\boldsymbol{\phi}} H(\sum_c q_\phi(z|y{=}c)p(y{=}c))$
    $\mathbf{w}^{t+1}_{1:K} \leftarrow$ ADAM$(\Delta^t_{\mathbf{w}_{1:K}}, \beta)$
    $\boldsymbol{\phi}^{t+1} \leftarrow$ ADAM$(\Delta^t_{\boldsymbol{\phi}}, \beta)$
  end for
end function

function CLIENT SIDE$(s, \boldsymbol{\phi}, \mathbf{W})$
  Get local parameters θ_s
  for epoch e in $1, \ldots, E$ **do**
    for batch $b \in B$ **do**
      $q'_\phi(z|s), q_\phi(z|s) \leftarrow \mathbb{E}_{y \sim \mathcal{D}_s}[q_\phi(z|y)]$
      $q'_\phi(z = k|s) = 0$ if $q_\phi(z = k|s) < \eta/K$
      $q'_\phi(z|s) \leftarrow q'_\phi(z|s)/\sum_k q'_\phi(z = k|s)$
      $q'_\phi(z|y) \leftarrow q_\phi(z|y)$
      $q'_\phi(z = k|y) = 0$ if $q_\phi(z = k|s) < \eta/K$
      $q'_\phi(z|y) \leftarrow q'_\phi(z|y)/\sum_k q'_\phi(z = k|y)$
      $L_s \leftarrow \mathbb{E}_{q'_\phi(z|y_b)}[\log p_{\mathbf{w}_z}(y_b|\mathbf{x}_b, z)] +$
        $\mathbb{E}_{q_\phi(z|y_b)}[\log p_{\theta_s}(z|\mathbf{x}_b, s)]$
      $\boldsymbol{\phi} += \alpha \nabla_{\boldsymbol{\phi}} L_s$
      $\mathbf{W} += \alpha \nabla_{\mathbf{W}} L_s$
      $\theta_s += \alpha \nabla_{\theta_s} L_s$
    end for
  end for
  $q(z|s) \leftarrow \mathbb{E}_{y \sim \mathcal{D}_s}[q_\phi(z|y)]$
  $\mathbf{W}' \leftarrow [\mathbf{w}_k | q(z = k|s) \geq \eta/K]$
  $q'(z|s) \leftarrow q(z|s)$
  $q'(z = k|s) = 0$ if $q(z = k|s) < \eta/K$
  $q'(z|s) \leftarrow q'(z|s)/\sum_k q'(z = k|s)$ ▷ Renormalization
  return $\mathbf{W}'; \boldsymbol{\phi}; q'(z|s)$
end function