# OVERCOMING LABEL SHIFT IN TARGETED FEDERATED LEARNING

Anonymous authors

Paper under double-blind review

### ABSTRACT

Federated learning enables multiple actors to collaboratively train models without sharing private data. This unlocks the potential for scaling machine learning to diverse applications. Existing algorithms for this task are well-justified when clients and the intended target domain share the same distribution of features and labels, but this assumption is often violated in real-world scenarios. One common violation is label shift, where the label distributions differ across clients or between clients and the target domain, which can significantly degrade model performance. To address this problem, we propose FedPALS, a novel model aggregation scheme that adapts to label shifts by leveraging knowledge of the target label distribution at the central server. Our approach ensures unbiased updates under stochastic gradient descent, ensuring robust generalization across clients with diverse, labelshifted data. Extensive experiments on image classification demonstrate that Fed-PALS consistently outperforms standard baselines by aligning model aggregation with the target domain. Our findings reveal that conventional federated learning methods suffer severely in cases of extreme client sparsity, highlighting the critical need for target-aware aggregation. FedPALS offers a principled and practical solution to mitigate label distribution mismatch, ensuring models trained in federated settings can generalize effectively to label-shifted target domains.

### 1 INTRODUCTION

**031 032 033 034 035 036 037** Federated learning has become a prominent paradigm in machine learning, enabling multiple clients to collaboratively train models without sharing their data [\(Kairouz et al., 2021\)](#page-11-0). Central to this development is the widely-used *federated averaging* (FedAvg) algorithm, which aggregates model updates from clients, weighted by their data set sizes [\(McMahan et al., 2017\)](#page-12-0). This aggregation rule is well-justified when client data is independent and identically distributed (i.i.d.) and has been effective in diverse domains such as healthcare [\(Sheller et al., 2020\)](#page-12-1), finance risk prediction [\(Byrd](#page-10-0) [& Polychroniadou, 2020\)](#page-10-0), and natural language processing [\(Hilmkil et al., 2021\)](#page-11-1).

**038 039 040 041 042 043 044 045 046 047 048 049 050 051** The justification for FedAvg is weaker when clients exhibit systematic data heterogeneity, such as in the case of *label shift* [\(Zhao et al., 2018;](#page-13-0) [Woodworth et al., 2020\)](#page-13-1), since the learning objectives of clients differ from the objective optimized by the central server. Consider a federated learning task involving multiple retail stores (clients) where the goal is to predict the sales of different products based on customer purchase history, and deploy the trained model in a new store (target). Each store's sales reflect local preferences, leading to differences in label distributions and empirical risks. When label distributions vary substantially, the performance of FedAvg can be severely hampered [\(Karimireddy et al., 2020;](#page-11-2) [Zhao et al., 2018\)](#page-13-0). So, how can models be trained effectively across such heterogeneous clients? Several methods have been proposed to deal with client heterogeneity, such as regularization [\(Li et al., 2020a;](#page-11-3) [2021\)](#page-11-4), clustering [\(Ghosh et al., 2020;](#page-10-1) [Vardhan et al., 2024\)](#page-12-2), and meta-learning approaches [\(Chen et al., 2018;](#page-10-2) [Jiang et al., 2019;](#page-11-5) [Fallah et al., 2020a\)](#page-10-3). Still, these studies and prior work in federated learning assume that the target (or test) domain shares the same distribution as the combined training data from the clients. In many real-world applications, models must generalize to new target domains with different distributions and without training data.

**052 053** In the retail example, the target store has no individual transaction data available and is not involved in training the model. The challenge of generalizing under distributional domain shift without target data is not exclusive to federated learning but arises also in centralized settings [\(Blanchard et al.,](#page-10-4)

**054 055 056 057 058 059** [2011;](#page-10-4) [Muandet et al., 2013;](#page-12-3) [Ganin et al., 2016\)](#page-10-5). In centralized scenarios, domain adaptation techniques such as sample re-weighting [\(Lipton et al., 2018a\)](#page-11-6), or domain-invariant representations [\(Ar](#page-10-6)[jovsky et al., 2020\)](#page-10-6) can be employed to mitigate the effects of distributional shifts. However, these approaches require central access to observations from both the source and target domains. This is not feasible in federated learning due to the decentralized nature of the data. Neither the server nor the clients have access to both data sets, making direct application of these methods impractical.

**061 062 063 064 065 066 067 068 069 070 071 072 073** Contributions This work aims to improve the generalization of federated learning to target domains under *label shift*, in settings where the different label distributions of clients and target domains are known to the central server but unknown to the clients (see Section [2\)](#page-1-0). To address this problem, we propose a novel aggregation scheme called FedPALS that optimizes a convex combination of client models to ensure that the aggregated model is better suited for the label distribution of the target domain (Section [3.1\)](#page-3-0). Our approach is both well-justified and practical. We prove that the resulting stochastic gradient update behaves, in expectation, as centralized learning in the target domain (Proposition [1\)](#page-3-1), and examine its relation to standard federated averaging (Proposition [3.2\)](#page-4-0). We demonstrate the effectiveness of FedPALS through an extensive empirical evaluation (Section [5\)](#page-6-0), showing that it outperforms traditional approaches in scenarios where distributional shifts pose significant challenges. Moreover, we observe that traditional methods struggle particularly in scenarios where the training clients have sparse label distributions. As we show in Figures [2c](#page-8-0) and [5c](#page-16-0) in Section [5,](#page-6-0) performance drops sharply when a majority of labels are completely unrepresented in clients, highlighting the limitations of existing approaches under label shift with extreme client sparsity.

**074**

**060**

**075 076**

**101 102 103**

### <span id="page-1-0"></span>2 TARGETED FEDERATED LEARNING UNDER LABEL SHIFT

**077 078 079 080 081 082 083 084 085 086** Federated learning is a distributed machine learning paradigm wherein a global model  $h_{\theta}$  is trained at a central server by aggregating parameter updates from multiple clients [\(McMahan et al., 2017\)](#page-12-0). We focus on classification tasks in which the goal is for  $h_{\theta}$  to predict the most probable label  $Y \in \{1, ..., K\}$  for a given input  $X \in \mathcal{X}$ . Each client  $i = 1, ..., M$  holds a data set  $D_i = \{(x_{i,1}, y_{i,1}), ..., (x_{i,n_i}, y_{i,n_i})\}$  of  $n_i$  labeled examples. Due to privacy concerns or limited communication bandwidth, these data sets cannot be shared with other clients or with the central server. Learning proceeds over rounds  $t = 1, ..., t_{max}$ , each completing three steps: (1) The central server broadcasts the current global model parameters  $\theta_t$  to all clients; (2) Each client *i* computes updated parameters  $\theta_{i,t}$  based on their local data set  $D_i$  and sends these updates back to the server; (3) The server aggregates the clients' updates to obtain the new global model  $\theta_{t+1}$ .

**087 088 089 090 091 092 093 094** Client samples  $D_i$  are assumed to be drawn i.i.d. from a *local* client-specific distribution  $S_i(X, Y)$ . A common (implicit) assumption in federated learning is that the learned model will be applied in a target domain  $T(X, Y)$  that coincides with the marginal distribution of clients,  $\bar{S} = \sum_{i=1}^{M} \frac{n_i}{N} S_i$ , where  $N = \sum_{i=1}^{M} n_i$ . This is reflected in trained models being evaluated in terms of their average performance over all clients. In general, the target domain  $T(X, Y)$  may be distinct from both individual clients and their aggregate [\(Bai et al., 2024\)](#page-10-7). Moreover, clients may exhibit significant heterogeneity in their distributions,  $S_i \neq S_j$  [\(Karimireddy et al., 2020;](#page-11-2) [Li et al., 2020b\)](#page-11-7). We refer to this problem as *targeted federated learning*.

**095 096 097 098 099 100** We study targeted federated learning under known label shift, where no samples from the joint distribution  $T(X, Y)$  are available but the target label distribution  $T(Y)$  is known to the server. Let  $\mathcal{X} \subset \mathbb{R}^d$  denote the d-dimensional input space and  $\mathcal{Y} = \{1, ..., K\}$  the label space. Given a set of clients with distributions  $S_1, ..., S_M$  and a target domain with distribution T, our objective is to minimize the expected risk,  $R_T$  of a classifier  $h_\theta : \mathcal{X} \to \mathcal{Y}$ , with respect to a loss function  $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$  over the target distribution T,

<span id="page-1-1"></span>
$$
\underset{\theta}{\text{minimize}} R_T(h_{\theta}) \coloneqq \mathop{\mathbb{E}}_{(X,Y)\sim T} \left[ \ell(h_{\theta}(X), Y) \right]. \tag{1}
$$

**104 105 106 107** Obtaining a good estimate of  $T(Y)$  is often feasible since it represents aggregate statistics that can be collected without the need for a large dataset. In our retail example,  $Y = y$  would represent a sale in a specific product category, and  $T(y)$  would correspond to the proportion of total sales in that category. A company could estimate these proportions without logging customer features X. Our setting differs from domain generalization which lacks a specific target domain [\(Bai et al., 2024\)](#page-10-7).

**108 109 110 111 112 113 114 115 116 117** In our setting, the target and all client label distributions are all assumed distinct:  $\forall i \neq j \in [M]$ :  $S_i(Y) \neq S_j(Y) \neq T(Y)$ . Furthermore, the target distribution is assumed to differ from the client aggregate,  $T(Y) \neq \overline{S}(Y)$ . While the server has access to all marginal label distributions  $S_i(Y)_{i=1}^M$ and  $T(Y)$ , these are *not available to the clients*. For instance, most retailers would be hesitant to share their exact sales statistics  $T(Y)$  with competitors. Instead, they might provide this information to a neutral third party (central server) responsible for coordinating the federated learning process. More broadly, clients  $i \neq j$  do not communicate directly with each other but rather interact with the central server through model parameters. While it is technically possible for the server to *infer* each client's label distribution  $S_i(Y)$  based on their parameter updates (Ramakrishna & Dán, 2022), doing so would likely be considered a breach of trust in practical applications.

**118 119** The distributional shifts between clients and the target are restricted to *label shift*—while the label distributions vary across clients and the target, the class-conditional input distributions are identical.

<span id="page-2-1"></span>**120 121 Assumption 1** (Label shift). *For the client distributions*  $S_1, ..., S_M$  *and the target distribution*  $T$ ,

$$
\forall i, j \in [M] : S_i(X \mid Y) = S_j(X \mid Y) = T(X \mid Y).
$$
 (2)

**122 123**

**124 125 126 127 128 129 130 131 132 133** This setting has been well studied in non-federated learning, both in cases where the label marginals are known and where they are not [\(Lipton et al., 2018b\)](#page-11-8). In the retail example, label shift would mean that while the proportion of sales across product categories  $(S_i(Y)$  and  $T(Y))$  varies between different retailers and the target, the purchasing patterns within each category  $(S_i(X \mid Y)$  and  $T(X | Y)$  remain consistent. In other words, although retailers may sell different quantities of products across categories, the characteristics of customers buying a particular product (conditional on the product category) are assumed to be the same. Note that there are settings where both the label shift and *covariate shift* assumptions hold, that is  $\forall i : S_i(Y \mid X) = T(Y \mid X)$  and  $S_i(X \mid X)$  $Y = T(X | Y)$ , but  $S_i(X), T(X)$  differ, such as when the labeling function is deterministic. We do not consider general covariate shift (without the label shift assumption) here.

**Our central question is:** In federated learning, how can we *aggregate* the parameter updates  $\theta_{i,t}$ of the M clients, whose data sets are drawn from distributions  $S_1, ..., S_M$ , such that the resulting federated learning algorithm minimizes the target risk,  $R_T$ ? The fact that clients are ignorant of the shift in  $T(Y)$  affects the optimal strategy; direct access to  $T(Y)$  would allow sample re-weighting or upsampling in the client objectives [\(Rubinstein & Kroese, 2016\)](#page-12-5). This is not possible here.

**138 139 140**

**161**

### 3 FEDPALS: PARAMETER AGGREGATION TO ADJUST FOR LABEL SHIFT

In classical federated learning, all clients and the target domain are assumed i.i.d., and thus, the target risk (equation [1\)](#page-1-1) is equal to the expected risk in any client

$$
R_T(h) = \mathop{\mathbb{E}}_{(X,Y) \sim S_i} [\ell(h(X),Y)] =: R_i(h), \text{ for all } i = 1,...,M .
$$

Similarly, the empirical risk  $\hat{R}_i$  of any client i is identical in distribution (denoted  $\stackrel{d}{=}$ ) to the empirical risk evaluated on a hypothetical data set  $D_T = \{(x_{T,j}, y_{T,j})\}_{j=1}^{n_T}$  drawn from the target domain,

$$
\hat{R}_i := \frac{1}{n_i} \sum_{j=1}^{n_i} \ell(h(x_{i,j}), y_{i,j}) \stackrel{d}{=} \frac{1}{n_T} \sum_{j=1}^{n_T} \ell(h(x_{T,j}), y_{T,j}) =: \hat{R}_T
$$

As a result, if clients perform a single local gradient descent update, any convex combination of these gradients (updates) is equal in distribution to a classical (centralized) batch update for the target domain, given the previous parameter value,

$$
\forall \alpha \in \Delta^{M-1} : \sum_i \alpha_i \nabla_{\theta} \hat{R}_i(h_{\theta}) \stackrel{d}{=} \nabla_{\theta} \hat{R}_T(h_{\theta}),
$$

**159 160** where  $\Delta^{M-1} = \{ \alpha \in [0,1]^M : \sum_i \alpha_i = 1 \}$  is the simplex over M elements. This property justifies the federated stochastic gradient (FedSGD) and FedAvg principles [\(McMahan et al., 2017\)](#page-12-0),<sup>[1](#page-2-0)</sup> which

<span id="page-2-0"></span><sup>&</sup>lt;sup>1</sup> Strictly speaking, only FedSGD uses the property directly, but FedAvg is a natural extension.

**162 163** aggregate model parameter updates through a convex combination, chosen to give weight to clients proportional to their sample size,

**164 165**

**166 167**

**173 174 175**

**178 179 180**

$$
\theta_{t+1}^{FA} = \sum_{i=1}^{M} \alpha_i^{FA} \theta_{i,t} \quad \text{where} \quad \alpha_i^{FA} = \frac{n_i}{\sum_{j=1}^{M} n_j} \,. \tag{3}
$$

**168 169 170 171 172** A limitation of FedAvg aggregation is that when client and target domains are not identically distributed, and  $T \neq \bar{S}$ ,  $\{\nabla \hat{R}_i\}_{i=1}^M$  are no longer unbiased estimates of the risk gradient in the target domain,  $\nabla R_T$ . As a result, the FedAvg update is not an unbiased estimate of a model update computed in the target domain. As we see in Table [1](#page-7-0) in section [5,](#page-6-0) this can have large effects on model quality.

### <span id="page-3-0"></span>3.1 OVERCOMING LABEL SHIFT WHILE CONTROLLING VARIANCE

**176 177** Next, we develop an alternative aggregation strategy that partially overcomes the limitations of FedAvg under *label shift* (Assumption [1\)](#page-2-1). Under label shift, it holds that

$$
\forall i: R_T(h) = \sum_{y=1}^K T(y) \int_x \underbrace{T(x \mid y)}_{=S_i(x \mid y)} \ell(h(x), y) dx = \sum_{y=1}^K T(y) \mathbb{E}_{S_i} [\ell(h(X), y) \mid Y = y].
$$

**181 182 183 184 185** In centralized (non-federated) learning under label shift, this insight is often used to re-weight [\(Lip](#page-11-8)[ton et al., 2018b\)](#page-11-8) or re-sample [\(Japkowicz & Stephen, 2002\)](#page-11-9) the empirical risk in the source domain. *This is not an option here since*  $T(Y)$  *is not revealed to the clients.* For now, assume instead that the target label distribution can be covered by a convex combination of client label distributions. For this, let  $Conv(S)$  denote the convex hull of distributions  $\{S_i(Y)\}_{i=1}^M$ .

<span id="page-3-2"></span>**186 187 188 Assumption 2** (Target coverage). *For the label marginals*  $S_1(Y), ..., S_M(Y), T(Y) \in \Delta^{K-1}$ , the *target label distribution*  $T(Y)$  *is covered by a convex combination*  $\alpha^c$  *of client label distributions,* 

<span id="page-3-3"></span>
$$
T \in Conv(S), \quad i.e., \quad \exists \alpha^c \in \Delta^{M-1} : T(y) = \sum_{i=1}^M \alpha_i^c S_i(y) \quad \forall y \in [K]. \tag{4}
$$

Note that, under label shift, Assumption [2](#page-3-2) implies that  $T(X,Y) = \sum_{i=1}^{M} \alpha_i^c S_i(X,Y)$ , as well. Thus, under Assumptions [1–](#page-2-1)[2,](#page-3-2) we have for any  $\alpha^c$  satisfying equation [4,](#page-3-3)

$$
R_T(h) = \sum_{y=1}^{K} \left( \sum_{i=1}^{M} \alpha_i^c S_i(y) \right) \mathbb{E}[\ell(h(X), y) | Y = y] = \sum_{i=1}^{M} \alpha_i^c R_{S_i}(h).
$$
 (5)

<span id="page-3-1"></span>By extension, aggregating client updates with weights  $\alpha^c$  will be an unbiased estimate of the update. Proposition 1 (Unbiased SGD update). *Consider a single round* t *of federated learning in the batch stochastic gradient setting with learning rate*  $\eta$ . Each client  $i \in [M]$  *is given parameters*  $\theta_t$  *by the server, computes their local gradient, and returns the update*  $\theta_{i,t} = \theta_t - \eta \nabla_\theta \hat{R}_i(h_{\theta_t})$ . Let weights  $\alpha^c$  satisfy  $T(X,Y) = \sum_{i=1}^M \alpha_i^c S_i(X,Y)$ . Then, the aggregate update  $\theta_{t+1} = \sum_{i=1}^M \alpha_i^c \theta_{i,t}$  satisfies  $\mathbb{E}[\theta_{t+1} | \theta_t] = \mathbb{E}[\theta_{t+1}^T | \theta_t],$ 

where  $\theta^T_{t+1}=\theta_t-\eta\nabla_\theta \hat{R}_T(h_{\theta_t})$  is the batch stochastic gradient descent (SGD) update for  $\hat{R}_T$  that *would be obtained with a sample from the target domain. A proof is given in Appendix [C.](#page-18-0)*

By Proposition [1,](#page-3-1) we are justified<sup>[2](#page-3-4)</sup> in replacing the aggregation step of FedAvg with one where clients are weighted by  $\alpha^c$ . However, Assumption [2](#page-3-2) may not hold, and  $\alpha^c$  may not exist. For instance, if the target marginal is sparse, only clients with *the exact same sparsity pattern* as T can be used in a convex combination  $\alpha^c S = T$ . That is, if we aim to classify images of animals and T contains no tigers, then no clients contributing to the combination can have data containing tigers. At least, since  $\{\tilde{S}_i(Y)\}_{i=1}^M$ ,  $T(Y)$  are known to the server, it is straightforward to verify Assumption [2.](#page-3-2)

<span id="page-3-4"></span><sup>&</sup>lt;sup>2</sup>Note that, just like in FedAvg, aggregating client parameter updates resulting from multiple local stochastic gradient steps (e.g., one epoch) is not guaranteed to locally minimize the target risk.

<span id="page-4-4"></span><span id="page-4-1"></span>

**228 229 230** Figure 1: Illustration of the target label marginal T and client marginals  $S_1, ..., S_4$  in a ternary classification task,  $Y \in \{0, 1, 2\}$ . Left: there are fewer clients than labels,  $M < K$ , and  $T \notin \{0, 1, 2\}$ . Conv(S);  $\alpha^0 S$  is a projection of T onto Conv(S). Right:  $T \in Conv(S)$  and coincides with  $\alpha^0 S$ . In both cases, the label marginal  $\alpha^{FA}S$  implied by FedAvg is further from the target distribution.

Remark. In practice, many federated learning systems, including FedAvg, allow clients to perform several steps of local optimization (e.g., over an entire epoch) before aggregating the parameter updates at the server. This is a limitation of Proposition [1:](#page-3-1) when clients are not constrained to a single SGD step, the aggregated updates no longer strictly minimize the target risk.

A pragmatic choice when Assumption [2](#page-3-2) is violated is to look for the convex combination  $\alpha^0$  that most closely aligns with the target label distribution, and use that in the aggregation step,

<span id="page-4-2"></span>
$$
\alpha^0 = \underset{\alpha \in \Delta^{M-1}}{\arg \min} \left\| \sum_{i=1}^M \alpha_i S_i(Y) - T(Y) \right\|_2^2 \quad \text{and} \quad \theta_{t+1}^0 = \sum_i \alpha_i^0 \theta_{i,t} \,. \tag{6}
$$

We illustrate the label distributions implied by weighting with  $\alpha^0$  and  $\alpha^{FA}$  (FedAvg) in Figure [1.](#page-4-1)

**244 245 246 247 248 249 250 251 252 253 Effective sample size of aggregates.** A limitation of aggregating using  $\alpha^0$  as defined in equation [6](#page-4-2) is that, unlike FedAvg, it does not give higher weight to clients with larger sample sizes, which can lead to a higher variance in the model estimate. The variance of importance-weighted estimators can be quantified through the concept of *effective sample size* (ESS) [\(Kong, 1992\)](#page-11-10), which measures the number of samples needed from the target domain to achieve the same variance as a weighted estimate computed from source-domain samples. ESS is often approximated as  $1/(\sum_{i=1}^m w_i^2)$  where w are normalized sample weights such that  $w_j \ge 0$  and  $\sum_{j=1}^n w_j = 1$ . In federated learning, we can interpret the aggregation step as assigning a total weight  $\alpha_i$  to each client i, which has  $n_i$  samples. Consequently, each sample  $(x_j, y_j) \in D_i$  has the same weight  $\tilde{w}_j = \alpha_i/n_i$ . The ESS for the aggregate is then given by  $1/(\sum_{i=1}^{m}(\sum_{j \in S_i} \tilde{w}_j^2)) = 1/(\sum_{i=1}^{m} n_i \alpha_i^2/n_i^2) = 1/(\sum_{i=1}^{m} \alpha_i^2/n_i).$ 

**254 256** In light of the results above, we propose a client aggregation step such that the weighting of clients' label distributions will a) closely align with the target label distribution, and b) minimize the variance due to weighting using the inverse of the ESS. For a given regularization parameter  $\lambda \in [0, \infty)$ , we define a weighting scheme  $\alpha^{\lambda}$  as the solution to the following problem.

<span id="page-4-3"></span>
$$
\alpha^{\lambda} = \underset{\alpha \in \Delta^{M-1}}{\arg \min} ||T(Y) - \sum_{i=1}^{M} \alpha_i S_i(Y)||_2^2 + \lambda \sum_{i} \frac{\alpha_i^2}{n_i}, \qquad (7)
$$

and aggregate client parameters inside federated learning as  $\theta_{t+1}^{\lambda} = \sum_{i=1}^{M} \alpha_i^{\lambda} \theta_{i,t}$ . We refer to this strategy as Federated learning with Parameter Aggregation for Label Shift (FedPALS).

### <span id="page-4-0"></span>3.2 FEDPALS IN THE LIMITS

**255**

**267 268 269** In the FedPALS aggregation scheme (equation [7\)](#page-4-3), there exists a trade-off between closely matching the target label distribution and minimizing the variance of the model parameters. This trade-off gives rise to two notable limit cases:  $T \in Conv(S), \lambda \to 0$ , and  $\lambda \to \infty$ . If all source distributions  $\{S_i\}_{i=1}^M$  are identical and match the target distribution, this corresponds to the classical i.i.d. setting.

**270 271 272 Case 1:**  $\lambda \to \infty$   $\Rightarrow$  **Federated averaging** In the limit  $\lambda \to \infty$ , as the regularization parameter  $\lambda$ grows large, FedPALS aggregation approaches FedAvg aggregation.

**273 Proposition 2.** The limit solution  $\alpha^{\lambda}$  to equation [7,](#page-4-3) as  $\lambda \to \infty$ , is

$$
\lim_{\lambda \to \infty} \alpha_i^{\lambda} = \frac{n_i}{\sum_{j=1}^M n_j} = \alpha_i^{FA} \quad \text{for} \quad i = 1, \dots, M \,. \tag{8}
$$

**276 277 278 279 280** The result is proven in Appendix [C.](#page-18-0) By Proposition [2,](#page-4-4) the FedAvg weights  $\alpha^{FA}$  minimize the ESS and coincide with FedPALS weights  $\alpha^{\lambda}$  in the limit  $\lambda \to \infty$ . As a rare special case, whenever  $T(Y) = \overline{S} = \sum_{i=1}^{M} \frac{n_i}{N} S_i(Y)$ , FedAvg weights  $\alpha^{FA} = \alpha^{\lambda}$  for any value of  $\lambda$ , since both terms attain their mimima at this point. However, this violates the assumption that  $T(Y) \neq \overline{S}(Y)$ .

**281 282 283 284 285 286 287 288 Case 2: Covered target,**  $T \in Conv(S)$  Now, consider when the target label distribution is in the convex hull of the source label distributions,  $Conv(S)$ . Then, we can find a convex combination  $\alpha^c$ of source distributions  $S_i(Y)$  that recreate  $T(Y)$ , that is,  $T(Y) = \sum_{i=1}^{M} \alpha_i^c S_i(Y)$ . However, when there are more clients than labels,  $M > K$ , such a *satisfying combination*  $\alpha^c$  need not be unique and different combinations may have different effective sample size. Let  $A^c = \{ \alpha^c \in \Delta^{M-1} : T(Y) =$  $(\alpha^c)^\top S(Y)$  denote all satisfying combinations where  $S(Y) \in \mathbb{R}^{M \times K}$  is the matrix of all client label marginals. For a sufficiently small regularization penalty  $\lambda$ , the solution to equation [7](#page-4-3) will be the satisfying combination with largest effective sample size.

**289**

**274 275**

**290 291**

**299**

 $\lim_{\lambda \to 0} \alpha^{\lambda} = \argmin_{\alpha \in A^c}$  $\sum^M$  $i=1$  $\alpha_i^2$  $\frac{a_i}{n_i}$ .

**292 293 294 295** If there are fewer clients than labels,  $M < K$ , the set of target distributions for which a satisfying combination exists has measure zero, see Figure [1](#page-4-1) (left). Nevertheless, the two cases above allow us to interpolate between being as faithful as possible to the target label distribution ( $\lambda \to 0$ ) and retaining the largest effective sample size ( $\lambda \to \infty$ ), the latter coinciding with FedAvg.

**296 297 298** Finally, when  $T \in Conv(S)$  and  $\lambda \to 0$ , Proposition [1](#page-3-1) applies also to FedPALS; the aggregation strategy results in an unbiased estimate of the target risk gradient in the SGD setting. However, like the unregularized weights, Proposition [1](#page-3-1) does not apply for multiple local client updates.

**300 301 302 Case 3:**  $T \notin Conv(S)$  If the target distribution does not lie in Conv(S), see Figure [1](#page-4-1) (left), FedPALS projects the target to the "closest point" in  $Conv(S)$  if  $\lambda = 0$ , and to a tradeoff between this projection and the FedAvg aggregation if  $\lambda > 0$ .

**303 304 305 306 307 308 309 310 311 312 313 314 315 Choice of hyperparameter**  $\lambda$  A salient question in Cases 2 & 3 is how to choose the strength of the regularization,  $\lambda$ . A larger value will generally favor influence from more clients, provided that they have sufficiently many samples. When  $T \notin Conv(S)$ , the convex combination closest to T could have weight on a single vertex. This will likely hurt the generalizability of the resulting classifier. In experiments, we compare values of  $\lambda$  that yield different effective sample sizes, such as 10%, 25%, 50%, 75%, or 100% of the original sample size, N. We can find these using binary search by solving equation [7](#page-4-3) and calculate the ESS. One could select  $\lambda$  heuristically based on the the ESS, or treat  $\lambda$  as a hyperparameter and select it using a validation set. Although this would entail training and evaluating several models which can be seen as a limitation. We elect to choose a small set of  $\bar{\lambda}$  values based on the ESS heuristic and train models for these. Then we use a validation set to select the best performing model. This highlights the usefulness of the ESS as a heuristic. If it is unclear which values to pick, one could elect for a simple strategy of taking the ESS of  $\lambda = 0$  and 100% and taking  $l$  equidistributed values in between the two extremes, for some small integer  $l$ .

**316 317 318 319 320 321 322 323 Sparse clients and targets** In problems with a large number of labels,  $K \gg 1$ , it is common that any individual domain (clients or target) supports only a subset of the labels. For example, in the IWildCam benchmark, not every wildlife camera captures images of all animal species. When the target  $T(Y)$  is *sparse*, meaning  $T(y) = 0$  for certain labels y, it becomes easier to find a good match  $({\alpha}^{\bar{\lambda}})^{\top} S(Y) \approx T(Y)$  if the client label distributions are also sparse. Achieving a perfect match, i.e.,  $T \in Conv(S)$ , requires that (i) the clients collectively cover all labels in the target, and (ii) each client contains only labels that are present in the target. If this is also beneficial for learning, it would suggest that the client-presence of labels that are not present in the target would *harm* the aggregated model. We study the implications of sparsity of label distributions empirically in Section [5.](#page-6-0)

#### **324** 4 RELATED WORK

**325 326**

**327 328 329 330 331 332 333 334 335 336 337 338** Efforts to mitigate the effects of distributional shifts in federated learning can be broadly categorized into client-side and server-side approaches. Client-side methods use techniques such as clustering clients with similar data distributions and training separate models for each cluster [\(Ghosh et al.,](#page-10-1) [2020;](#page-10-1) [Sattler et al., 2020;](#page-12-6) [Vardhan et al., 2024\)](#page-12-2), and meta-learning to enable models to quickly adapt to new data distributions with minimal updates [\(Chen et al., 2018;](#page-10-2) [Jiang et al., 2019;](#page-11-5) [Fallah](#page-10-8) [et al., 2020b\)](#page-10-8). Other notable strategies include logit calibration [\(Zhang et al., 2022\)](#page-13-2), regularization techniques that penalize large deviations in client updates to ensure stable convergence [\(Li et al.,](#page-11-7) [2020b;](#page-11-7) [2021\)](#page-11-4), and recent work on optimizing for flatter minima to enhance model robustness [\(Qu](#page-12-7) [et al., 2022;](#page-12-7) [Caldarola et al., 2022\)](#page-10-9). Server-side methods focus on improving model aggregation or applying post-aggregation adjustments. These include optimizing aggregation weights [\(Reddi et al.,](#page-12-8) [2021\)](#page-12-8), learning adaptive weights [\(Li et al., 2023\)](#page-11-11), iterative moving averages to refine the global model [\(Zhou et al., 2023\)](#page-13-3), and promoting gradient diversity during updates [\(Zeng et al., 2023\)](#page-13-4). Both categories of work overlook shifts in the target distribution, leaving this area unexplored.

**339 340 341 342 343 344 345 346 347** Another related area is personalized federated learning, which focuses on fine-tuning models to optimize performance on each client's specific local data [\(Collins et al., 2022;](#page-10-10) [Boroujeni et al., 2024;](#page-10-11) [Fallah et al., 2020a\)](#page-10-3). This setting differs fundamentally from our work, which focuses on improving generalization to new target clients without any training data available for fine-tuning. Label distribution shifts have also been explored with methods such as logit calibration [\(Zhang et al., 2022;](#page-13-2) [Wang et al., 2023;](#page-12-9) [Xu et al., 2023\)](#page-13-5), novel loss functions [\(Wang et al., 2021\)](#page-12-10), feature augmentation [\(Xia et al., 2023\)](#page-13-6), gradient reweighting [\(Xiao et al., 2023\)](#page-13-7), and contrastive learning [\(Wu et al.,](#page-13-8) [2023\)](#page-13-8). However, like methods aimed at mitigating the effects of general shifts, these do not address the challenge of aligning models with an unseen target distribution, as required in our setting.

**348 349 350 351 352 353 354 355 356** Generalization under domain shift in federated learning remains underdeveloped [\(Bai et al., 2024\)](#page-10-7). The work most similar to ours is that of agnostic federated learning (AFL) [\(Mohri et al., 2019\)](#page-12-11), which aims to learn a model that performs robustly across all possible target distributions within the convex hull of client distributions. One notable approach is tailored for medical image segmentation, where clients share data in the frequency domain to achieve better generalization across domains [\(Liu et al., 2021\)](#page-12-12). However, this technique requires data sharing, making it unsuitable for privacy-sensitive applications like ours. A different line of work focuses on addressing covariate shift in federated learning through importance weighting [\(Ramezani-Kebrya et al., 2023\)](#page-12-13). Although effective, this method requires sending samples from the test distribution to the server, which violates our privacy constraints.

**357 358**

**359 360**

## <span id="page-6-0"></span>5 EXPERIMENTS

**361 362 363 364 365 366** We perform a series of experiments on benchmark data sets to evaluate FedPALS in comparison with baseline federated learning algorithms. The experiments aim to demonstrate the value of the central server knowing the label distributions of the client and target domains when these differ substantially. Additionally, we seek to understand how the parameter  $\lambda$ , controlling the trade-off between bias and variance in the FedPALS aggregation scheme, impacts the results. Finally, we investigate how the benefits of FedPALS are affected by the sparsity of label distributions and by the distance  $d(T, S) := \min_{\alpha \in \Delta^{M-1}} ||T(Y) - \alpha^{\top} S(Y)||_2^2$  from the target to the convex hull of clients.

**367 368**

**369 370 371 372 373 374 375 376 377** Experimental setup While numerous benchmarks exist for federated learning [\(Caldas et al., 2018;](#page-10-12) [Ogier du Terrail et al., 2022;](#page-12-14) [Chen et al., 2022\)](#page-10-13) and domain generalization [\(Gulrajani & Lopez-Paz,](#page-10-14) [2020;](#page-10-14) [Koh et al., 2021\)](#page-11-12), respectively, until recently none have addressed tasks that combine both settings. To fill this gap, [Bai et al.](#page-10-7) [\(2024\)](#page-10-7) introduced a benchmark specifically designed for federated domain generalization (DG), evaluating methods across diverse datasets with varying levels of client heterogeneity. In our experiments, we use the PACS [Li et al.](#page-11-13) [\(2017\)](#page-11-13) and iWildCAM data sets from the [Bai et al.](#page-10-7) [\(2024\)](#page-10-7) benchmark to model realistic label shifts between the client and target distributions. We modify the PACS dataset to consist of three clients, each missing a label that is present in the other two. Additionally, one client is reduced to one-tenth the size of the others, and the target distribution is made sparse in the same label as that of the smaller client. Further details are given in Appendix [A.](#page-14-0)

<span id="page-7-0"></span>**378 379 380 381 382** Table 1: Comparison of mean accuracy and standard deviation  $(\pm)$  across different algorithms. The reported values are over 8 independent random seeds for the CIFAR-10 and Fashion-MNIST tasks, and 3 for PACS. C indicates the number of labels per client and  $\beta$  the Dirichlet concentration parameter. M is the number of clients. The *Oracle* method refers to a FedAvg model trained on clients whose distributions are identical to the target.

Data set	Label split	M	FedPALS	FedAvg	FedProx	<b>SCAFFOLD</b>	AFL	Oracle
Fashion-MNIST	$C=3$ $C=2$	10	$92.4 + 2.1$ $80.6 + 23.7$	$67.1 + 22.0$ $53.9 + 36.2$	$66.9 + 20.8$ $52.9 + 35.7$	$69.5 \pm 19.3$ $54.9 \pm 36.8$	$72.2 + 16.5$ $72.8 \pm 21.7$	$97.6 + 2.1$ $97.5 + 4.0$
$CIFAR-10$	$C=3$ $C=2$ $\beta = 0.1$	10	$65.6 + 10.1$ $72.8 + 17.4$ $62.6 + 17.9$	$44.0 + 8.4$ $46.7 + 15.8$ $40.8 + 9.2$	$43.5 + 7.2$ $47.7 + 15.6$ $41.9 + 9.7$	$43.3 + 7.4$ $46.7 + 14.9$ $43.5 + 10.5$	$53.2 + 0.9$ $54.7 + 0.1$ $53.4 + 11.5$	$85.5 + 5.0$ $89.2 + 3.9$ $79.2 + 3.7$
<b>PACS</b>	$C=6$		$86.0 + 2.9$	$73.4 + 1.6$	$75.3 + 1.3$	$73.9 \pm 0.3$	$74.5 + 0.9$	$90.5 + 0.3$

> Furthermore, we construct two additional tasks by introducing label shift to standard image classification data sets, Fashion-MNIST [\(Xiao et al., 2017\)](#page-13-9) and CIFAR-10 [\(Krizhevsky, 2009\)](#page-11-14). We apply two label shift sampling strategies: sparsity sampling and Dirichlet sampling. Sparsity sampling involves randomly removing a subset of labels from clients and the target domain, following the data set partitioning technique first introduced in [McMahan et al.](#page-12-0) [\(2017\)](#page-12-0) and extensively used in subsequent studies [\(Geyer et al., 2017;](#page-10-15) [Li et al., 2020a;](#page-11-3) [2022\)](#page-11-15). Each client is assigned C random labels, with an equal number of samples for each label and no overlap among clients.

**398 399 400 401 402 403 404 405 406 407** Dirichlet sampling simulates realistic non-i.i.d. label distributions by, for each client  $i$ , drawing a sample  $p_i \sim$  Dirichlet $_K(\beta)$ , where  $p_i(k)$  represents the proportion of samples in client i that have label  $k \in [K]$ . We use a symmetric concentration parameter  $\beta > 0$  which controls the sparsity of the client distributions. A smaller  $\beta$  results in more heterogeneous client data sets, while a larger value approximates an i.i.d. setting. This widely-used method for sampling clients was first introduced by [Yurochkin et al.](#page-13-10) [\(2019\)](#page-13-10). While prior works have focused on inter-client distribution shifts assuming that client and target domains are equally distributed, *we apply these sampling strategies also to the target set*, thereby introducing label shift between the client and target data. Figures [2b](#page-8-0) & [5b](#page-16-0) (latter in appendix) illustrate an example with  $C = 6$  for sparsity sampling and Dirichlet sampling with  $\beta = 0.1$ , where the last client (Client 9) is chosen as the target. In addition, we investigate the effect of  $T(Y) \notin Conv(S)$  in a synthetic task described in [B.4.](#page-17-0)

**408**

**409 410 411 412 413 414 415 416 417 418 419 420 421 422 423** Baseline algorithms and model architectures Alongside FedAvg, we use SCAFFOLD, FedProx and AFL [\(Karimireddy et al., 2020;](#page-11-2) [Li et al., 2020b;](#page-11-7) [Mohri et al., 2019\)](#page-12-11) as baselines, the first two chosen due to their prominence in the literature and AFL as it is similar in nature to FedPALS. SCAFFOLD mitigates client drift in heterogeneous data environments by introducing control variates to correct local updates. FedProx incorporates a proximal term to the objective to limit the divergence of local models from the global model. AFL optimizes the global model to perform well on an unknown target which is a combination of the clients. For the synthetic experiment in Section [B.4,](#page-17-0) we use a logistic regression model. For CIFAR-10 and Fashion-MNIST, we use small, two-layer convolutional networks, while for PACS and iWildCAM, we use a ResNet-50 pre-trained on ImageNet. Early stopping, model hyperparameters, and  $\lambda$  in FedPALS are tuned using a validation set that reflects the target distribution in the synthetic experiment, CIFAR-10, Fashion-MNIST, and PACS. This tuning process consistently resulted in setting the number of local epochs to  $E = 1$ across all experiments. For iWildCAM, we adopt the hyperparameters reported by [Bai et al.](#page-10-7) [\(2024\)](#page-10-7) and select  $\lambda$  using the same validation set used in their work. We report the mean test accuracy and standard deviation for each method over 3 independent random seeds for PACS and iWildCam and 8 seeds for the smaller Fashion-MNIST and CIFAR-10, to ensure a robust evaluation.

**424 425**

**426**

### 5.1 EXPERIMENTAL RESULTS ON BENCHMARK TASKS

**427 428 429 430 431** We present summary results for three tasks with selected skews in Table [1](#page-7-0) and explore detailed results below. Across these tasks, FedPALS consistently outperforms or matches the best-performing baseline. For PACS, Fashion-MNIST and CIFAR-10, we include results for an *Oracle* FedAvg model, which is trained on clients whose distributions are identical to the target distribution, eliminating any client-target distribution shift (see Appendix [A](#page-14-0) for details on its construction). A Fed-PALS *Oracle* would be equivalent since there is no label shift. The *Oracle*, which enjoys perfect

<span id="page-8-0"></span>

tween target and client convex hull, varying C. with  $C = 6$  labels per client.

 $(c)$  Accuracy vs labels per client,  $C$ .

Figure 2: Results on CIFAR-10 with sparsity sampling, varying the number of labels per clients  $C$ across 10 clients. Clients with IDs 0–8 are used in training, and Client 9 is the target client. The task is more difficult for small  $C$ , when fewer clients share labels, and the projection distance is larger.

<span id="page-8-1"></span>

Figure 3: Target accuracy during training of FedPALS compared to baselines on PACS (a) and iWildCam (b), averaged over 3 random seeds.  $M$  is the number of training clients.

alignment between client and target distributions, achieves superior performance, underscoring the challenges posed by distribution shifts in real-world scenarios where such alignment is absent.

**468 469 470 471 472 473 474 475 476** CIFAR-10/Fashion-MNIST. Figure [2c](#page-8-0) shows the results for the CIFAR-10 data set, where we vary the label sparsity across clients. In the standard i.i.d. setting, where all labels are present in both the training and target clients  $(C = 10)$ , all methods perform comparably. However, as label sparsity increases and fewer labels are available in client data sets (i.e., as C decreases), we observe a performance degradation in standard baselines. In contrast, our proposed method, FedPALS, leverages optimized aggregation to achieve a lower target risk, resulting in improved test accuracy under these challenging conditions. Similar trends are observed for Fashion-MNIST, as shown in Figure [6](#page-16-1) in Appendix [B.](#page-15-0) Furthermore, the results in the highly non-i.i.d. cases ( $C = 2, 3$  and  $\beta = 0.1$ ) are summarized in Table [1.](#page-7-0) Additional experiments in Appendix [B](#page-15-0) examine how the algorithms perform with varying numbers of local epochs and clients.

**477 478 479 480 481 482 483 484 485** PACS. As shown in Figure [3a,](#page-8-1) being faithful to the target distribution is crucial for improved performance. Lower values of  $\lambda$  generally correspond to better performance. Notably, FedAvg struggles in this setting because it systematically underweights the client with the distribution most similar to the target, leading to suboptimal model performance. In fact, this even causes performance to degrade over time. Interestingly, the baselines also face challenges on this task: both FedProx and SCAFFOLD perform similarly to FedPALS when  $\lambda = 93$ . However, FedPALS demonstrates significant improvements over these methods, highlighting the effectiveness of our aggregation scheme in enhancing performance. We also see that FedPALS + FedProx performs comparably to just using FedPALS in this case, although it does have higher variance. Additionally, in Table [1,](#page-7-0) we present the models selected based on the source validation set, where FedPALS outperforms all other methods.

**486 487 488** For comprehensive results, including all FedPALS models and baseline comparisons, please refer to Table [3](#page-15-1) in Appendix [B.](#page-15-0)

**489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505** iWildCam. The test performance across communication rounds is shown in Figure [3b.](#page-8-1) Initially, FedPALS widens the performance gap compared to FedAvg, but as training progresses, this gain diminishes. While FedPALS quickly reaches a strong performing model, it eventually plateaus. The rate of convergence and level of performance reached appears to be influenced by the choice of  $\lambda$ , with lower values of  $\lambda$  leading to faster plateaus at lower levels compared to larger ones. This suggests that more uniform client weights and a larger effective sample size are preferable in this task. Given the iWildCam dataset's significant class imbalance – with many classes having few samples – de-emphasizing certain clients can degrade performance. We also note that our assumption of label shift need not hold in this experiment, as the cameras are in different locations, potentially leading to variations in the conditional distribution  $p(X | Y)$ . The performance of the models selected using the source validation set is shown in Table [2](#page-15-2) in Appendix [B.](#page-15-0) There we see that FedPALS performs comparably to FedAvg and FedProx while outperforming SCAFFOLD. Unlike in other tasks, where FedProx performs comparably or worse than FedPALS, we see FedProx achieve the highest F1 score on this task. Therefore, we conduct an additional experiment where we use both FedProx and FedPALS together, as they are not mutually exclusive. This results in the best performing model, see Figure [3b.](#page-8-1) Finally, as an illustration of the impact of increasing  $\lambda$ , we provide the weights of the clients in this experiment alongside the FedAvg weights in [4](#page-15-3) in Appendix [B.](#page-15-0) We note that as  $\lambda$ increases, the weights increasingly align with those of FedAvg while retaining weight on the clients whose label distributions most resemble that of the target.

**506 507**

### 6 DISCUSSION

**508 509**

**510 511 512 513 514 515 516 517 518 519 520 521 522 523** We explored *targeted federated learning under label shift*, a scenario where client data distributions differ from a target domain with a known label distribution, but no target samples are available. We demonstrated that traditional approaches, such as FedAvg, which assume identical distributions between clients and the target, fail to adapt effectively in this context due to biased aggregation of client updates. To address this, we proposed FedPALS, a novel aggregation strategy that optimally combines client updates to align with the target distribution, ensuring that the aggregated model minimizes target risk. Empirically, across diverse tasks, we showed that under label shift, FedPALS significantly outperforms standard methods like FedAvg, FedProx and SCAFFOLD, as well as AFL. Specifically, when the target label distribution lies within the convex hull of the client distributions, FedPALS finds the solution with the largest effective sample size, leading to a model that is most faithful to the target distribution. More generally, FedPALS balances the trade-off between matching the target label distribution and minimizing variance in the model updates. Our experiments further highlight that FedPALS excels in challenging scenarios where label sparsity and client heterogeneity hinder the performance of conventional federated learning methods.

**524 525 526 527 528 529 530 531** We also observed that the choice of the trade-off parameter  $\lambda$  is crucial for achieving optimal performance in tasks such as iWildCam, where the label shift assumption may not fully hold. Moreover, FedPALS can underperform in scenarios where one or more clients, which are essential for accurately mirroring the target distribution, have limited sample sizes, and  $\lambda$  is set too low. In such cases, the effective sample size of the aggregated dataset becomes insufficient, potentially hindering the model's ability to learn effectively. Further, when the client aggregate is identical to the target, we do not expect this method to produce better solutions than FedAvg as the methods are equivalent in this case. Similar to many methods in FL there is an inherent privacy-accuracy trade-off where we achieve increased accuracy. However, this comes at the cost of clients sharing their label marginals.

**532 533 534 535 536 537 538 539** Interestingly, the early performance gains observed during training suggest that dynamically tuning  $\lambda$  over time could enhance performance of FedPALS. A promising avenue for future work would be exploring adaptive strategies for dynamically tuning  $\lambda$ . We also observed empirically that FedAvg tends to do much better when there is at least a small sample of each label in the clients making the gain from using FedPALS smaller. This could be further investigated to see if this behaviour can be replicated for more difficult tasks. Additionally, our weighting approach could be extended to the covariate shift setting, where input distributions vary between clients and the target. This extension is feasible when the central server has access to unlabeled target and client samples, akin to unsupervised domain adaptation in the centralized learning paradigm.

#### **540 541 REFERENCES**

<span id="page-10-15"></span><span id="page-10-14"></span><span id="page-10-13"></span><span id="page-10-12"></span><span id="page-10-11"></span><span id="page-10-10"></span><span id="page-10-9"></span><span id="page-10-8"></span><span id="page-10-7"></span><span id="page-10-6"></span><span id="page-10-5"></span><span id="page-10-4"></span><span id="page-10-3"></span><span id="page-10-2"></span><span id="page-10-1"></span><span id="page-10-0"></span>

<span id="page-11-15"></span><span id="page-11-14"></span><span id="page-11-13"></span><span id="page-11-12"></span><span id="page-11-11"></span><span id="page-11-10"></span><span id="page-11-9"></span><span id="page-11-8"></span><span id="page-11-7"></span><span id="page-11-6"></span><span id="page-11-5"></span><span id="page-11-4"></span><span id="page-11-3"></span><span id="page-11-2"></span><span id="page-11-1"></span><span id="page-11-0"></span>

- <span id="page-12-14"></span><span id="page-12-12"></span><span id="page-12-11"></span><span id="page-12-7"></span><span id="page-12-4"></span><span id="page-12-3"></span><span id="page-12-0"></span>**648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701** Quande Liu, Cheng Chen, Jing Qin, Qi Dou, and Pheng-Ann Heng. Feddg: Federated domain generalization on medical image segmentation via episodic learning in continuous frequency space. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 1013–1023, 2021. Brendan McMahan, Eider Moore, Daniel Ramage, Seth Hampson, and Blaise Aguera y Arcas. Communication-Efficient Learning of Deep Networks from Decentralized Data. In Aarti Singh and Jerry Zhu (eds.), *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics*, volume 54 of *Proceedings of Machine Learning Research*, pp. 1273–1282. PMLR, 20–22 Apr 2017. Mehryar Mohri, Gary Sivek, and Ananda Theertha Suresh. Agnostic federated learning. In Kamalika Chaudhuri and Ruslan Salakhutdinov (eds.), *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pp. 4615–4625. PMLR, 09–15 Jun 2019. Krikamol Muandet, David Balduzzi, and Bernhard Schölkopf. Domain generalization via invariant feature representation. In Sanjoy Dasgupta and David McAllester (eds.), *Proceedings of the 30th International Conference on Machine Learning*, volume 28 of *Proceedings of Machine Learning Research*, pp. 10–18, Atlanta, Georgia, USA, 17–19 Jun 2013. PMLR. Jean Ogier du Terrail, Samy-Safwan Ayed, Edwige Cyffers, Felix Grimberg, Chaoyang He, Regis Loeb, Paul Mangold, Tanguy Marchand, Othmane Marfoq, Erum Mushtaq, et al. Flamby: Datasets and benchmarks for cross-silo federated learning in realistic healthcare settings. *Advances in Neural Information Processing Systems*, 35:5315–5334, 2022. Zhe Qu, Xingyu Li, Rui Duan, Yao Liu, Bo Tang, and Zhuo Lu. Generalized federated learning via sharpness aware minimization. In *International conference on machine learning*, pp. 18250– 18280. PMLR, 2022. Raksha Ramakrishna and György Dán. Inferring class-label distribution in federated learning. In *Proceedings of the 15th ACM Workshop on Artificial Intelligence and Security*, pp. 45–56, 2022. Ali Ramezani-Kebrya, Fanghui Liu, Thomas Pethick, Grigorios Chrysos, and Volkan Cevher. Federated learning under covariate shifts with generalization guarantees. *Transactions on Machine Learning Research*, 2023. ISSN 2835-8856. Sashank Reddi, Zachary Burr Charles, Manzil Zaheer, Zachary Garrett, Keith Rush, Jakub Konečný, Sanjiv Kumar, and Brendan McMahan (eds.). *Adaptive Federated Optimization*, 2021. Reuven Y Rubinstein and Dirk P Kroese. *Simulation and the Monte Carlo method*. John Wiley & Sons, 2016. Felix Sattler, Klaus-Robert Müller, and Wojciech Samek. Clustered federated learning: Modelagnostic distributed multitask optimization under privacy constraints. *IEEE transactions on neural networks and learning systems*, 32(8):3710–3722, 2020. Micah J Sheller, Brandon Edwards, G Anthony Reina, Jason Martin, Sarthak Pati, Aikaterini Kotrotsou, Mikhail Milchenko, Weilin Xu, Daniel Marcus, Rivka R Colen, et al. Federated learning in medicine: facilitating multi-institutional collaborations without sharing patient data. *Scientific reports*, 10(1):12598, 2020. Harsh Vardhan, Avishek Ghosh, and Arya Mazumdar. An improved federated clustering algorithm with model-based clustering. *Transactions on Machine Learning Research*, 2024. Lixu Wang, Shichao Xu, Xiao Wang, and Qi Zhu. Addressing class imbalance in federated learning. *Proceedings of the AAAI Conference on Artificial Intelligence*, 35(11):10165–10173, May 2021. doi: 10.1609/aaai.v35i11.17219. Yuwei Wang, Runhan Li, Hao Tan, Xue Jiang, Sheng Sun, Min Liu, Bo Gao, and Zhiyuan Wu.
	- 13

<span id="page-12-13"></span><span id="page-12-10"></span><span id="page-12-9"></span><span id="page-12-8"></span><span id="page-12-6"></span><span id="page-12-5"></span><span id="page-12-2"></span><span id="page-12-1"></span>Federated skewed label learning with logits fusion. *ArXiv*, abs/2311.08202, 2023.

<span id="page-13-10"></span><span id="page-13-9"></span><span id="page-13-8"></span><span id="page-13-7"></span><span id="page-13-6"></span><span id="page-13-5"></span><span id="page-13-4"></span><span id="page-13-3"></span><span id="page-13-2"></span><span id="page-13-1"></span><span id="page-13-0"></span>

**758**

**APPENDIX** 

# <span id="page-14-0"></span>A EXPERIMENTAL DETAILS

Here we provide additional details about the experimental setup for the different tasks.

**763** A.1 ORACLE CONSTRUCTION

**764 765 766 767 768** The *Oracle* method serves as a benchmark to illustrate the performance upper bound when there is no distribution shift between the clients and the target. To construct this *Oracle*, we assume that the client label distributions are identical to the target label distribution, effectively eliminating the label shift that exists in real-world scenarios.

**769 770 771 772** In practice, this means that for each dataset, the client data is drawn directly from the same distribution as the target. The aggregation process in the *Oracle* method uses FedAvg, as no adjustments for label shift are needed. Since the client and target distributions are aligned, FedPALS would behave equivalently to FedAvg under this setting, as there is no need for reweighting the client updates.

**773 774 775 776** This method allows us to assess the maximum possible performance that could be achieved if the distributional differences between clients and the target did not exist. By comparing the *Oracle* results to those of our proposed method and other baselines, we can highlight the impact of label shift on model performance and validate the improvements brought by FedPALS.

- **777 778**
	- A.2 SYNTHETIC TASK

**779 780 781** We randomly sampled three means  $\mu_1 = [6, 4.6], \mu_2 = [1.2, -1.6],$  and  $\mu_3 = [4.6, -5.4]$  for each label cluster, respectively.

**782 783** A.3 PACS

**784 785 786 787 788 789 790 791** In this task we use the official source and target splits which are given in the work by [Bai et al.](#page-10-7) [\(2024\)](#page-10-7). We construct the task such that the training data is randomly assigned among three clients, then we remove the samples of one label from each of the clients. This is chosen to be labels '0', '1' and '2'. Then the client that is missing the label '2' is reduced so that it is 10% the amount of the original size. For the target we modify the given one by removing the samples with label '2', thereby making it more similar to the smaller client. To more accurately reflect the target distribution we modify the source domain validation set to also lack the samples with label '2'. This is reasonable since we assume that we have access to the target label distribution.

**792 793 794 795** We pick four values of  $\lambda$ , [0,12,42,93], which approximately correspond to an ESS of 15%, 25%, 50% and 75% respectively. We use the same hyperparameters during training as [Bai](#page-10-7) [et al.](#page-10-7) [\(2024\)](#page-10-7) report using in their paper. Furthermore, we use the cross entropy loss in this task.

**796 797** A.4 IWILDCAM

**798 799 800 801 802 803 804** We perform this experiment using the methodology described in [Bai et al.](#page-10-7) [\(2024\)](#page-10-7) with the heterogeneity set to the maximum setting, i.e.,  $\lambda = 0$  in their construction.<sup>[3](#page-14-1)</sup> We use the same hyperparameters which is used for FedAvg in the same work to train FedPALS. We perform 80 rounds of training and, we then select the best performing model based on held out validation performance and report the mean and standard deviation over three random seeds. This can be seen in Table [2.](#page-15-2) We pick four values of  $\lambda$ , [0,600,2500,5800], which approximately correspond to an ESS of 8%, 25%, 50% and 75% respectively. We use the cross entropy loss in this task.

**805 806 807 808** Due to FedProx performing comparably to FedPALS on this task, in contrast with other experiments, we also perform an experiment where we do both FedProx and FedPALS. This is easily done as FedProx is a client side method while FedPALS is a weighting method applied at the server. This results in the best performing model.

**<sup>809</sup>**

<span id="page-14-1"></span><sup>&</sup>lt;sup>3</sup>Note that this is not the same  $\lambda$  used in the trade-off in FedPALS.

**810 811** We use the same hyperparameters during training as [Bai et al.](#page-10-7) [\(2024\)](#page-10-7) report using in their paper. However, we set the amount of communication rounds to 80.

### <span id="page-15-0"></span>B ADDITIONAL EMPIRICAL RESULTS

Figure [4](#page-15-3) illustrates the aggregation weights of clients in the iWildCam experiment for  $\lambda$  corresponding to different effective sample sizes.

<span id="page-15-3"></span>

Figure 4: An illustration of the aggregation weights of clients in the iWildCam experiment using FedPALS for different ESS. The clients are sorted by amount of samples in descending order. The magnitude of the weights produced by federated averaging is shown as dots. Note that with increasing the ESS, the magnitudes more closely resemble that of federated averaging.

We report the performance of the models selected using the held out validation set in Table [2](#page-15-2) and Table [3](#page-15-1) for the iWildCam and PACS experiments respectively.

<span id="page-15-2"></span>Table 2: Results on iWildCam with 100 clients, standard deviation reported over 3 random seeds.



<span id="page-15-1"></span>



16

#### **864** B.1 RESULTS ON CIFAR-10 WITH DIRICHLET SAMPLING

**865 866 867**



<span id="page-16-0"></span>Figure [5](#page-16-0) shows the results for the CIFAR-10 experiment with Dirichlet sampling of client and target label distributions.

Figure 5: Results on CIFAR-10 with Dirichlet sampling across 10 clients, varying concentration parameter  $\beta$ . Clients with IDs 0–8 are clients present during training, and client with ID 9 is the target client.

<span id="page-16-1"></span>

Figure 6: Results on Fashion-MNIST with label sampling across 10 clients, varying parameter C. Clients with IDs 0–8 are clients present during training, and client with ID 9 is the target client.

### B.2 TRAINING DYNAMICS FOR FASHION-MNIST

Figure [7](#page-16-2) shows the training dynamics for Fashion-MNIST and CIFAR-10 with different label marginal mechanisms.

<span id="page-16-2"></span>



#### **918 919** B.3 LOCAL EPOCHS AND NUMBER OF CLIENTS

**960 961** In Figure [8c](#page-17-1) we show results for varying number of clients for each method. For the cases with number of clients 50 and 100, we use the standard sampling method of federated learning where a fraction of 0.1 clients are sampled in each communication round. In this case, we optimize  $\alpha^{\lambda}$  for the participating clients in each communication round. Interestingly, we observe that while FedAvg performs significantly worse than FedPALS on a target client under label shift, it outperforms both FedProx and SCAFFOLD when the number of local epochs is high ( $E = 40$ ), as shown in Figure [8b.](#page-17-1)

<span id="page-17-1"></span>

Figure 8: Comparison of CIFAR-10 results with different clients and settings. (a) 100 clients for  $C = 2, 3, 10, \lambda = 1000$ . (b) 10 clients and number of labels  $C = 3$ . We plot test accuracy as a function of number of local epochs  $E$ . The total number of communication rounds  $T$  are set such that  $T = E/150$ , where 150 is the number of rounds used for  $E = 1$ . (c) Test accuracy as a function of number of clients, with  $C = 3$ .

### <span id="page-17-0"></span>B.4 SYNTHETIC EXPERIMENT: EFFECT OF PROJECTION DISTANCE ON TEST ERROR

**946 947 948 949 950 951 952 953 954 955 956 957 958 959** When the target distribution  $T(Y)$  is not covered by the clients, FedPALS finds aggregation weights corresponding to a regularized projection of  $T$  onto  $Conv(S)$ . To study the impact of this, we designed a controlled experiment where the distance of the projection is varied. We create a classification task with three classes,  $\mathcal{Y} =$  $\{0, 1, 2\}$ , and define  $p(X \mid Y = y)$  for each label  $y \in Y$ by a unit-variance Gaussian distribution  $\mathcal{N}(\mu_y, I)$ , with randomly sampled means  $\mu_y \in \mathbb{R}^2$ . We simulate two clients with label distributions  $S_1(Y) = [0.5, 0.5, 0.0]^\top$ and  $S_2(Y) = [0.5, 0.0, 0.5]^\top$ , and  $n_1 = 40$ ,  $n_2 = 18$ samples, respectively. Thus, FedAvg gives larger weight to Client 1. We define a target label distribution  $T(Y)$  parameterized by  $\delta \in [0, 1]$  which controls the projection distance  $d(T, S)$  between  $T(Y)$  and  $Conv(S)$ ,

$$
T_{\delta}(Y) \coloneqq (1 - \delta) T_{\text{proj}}(Y) + \delta T_{\text{ext}}(Y) ,
$$

**962 963 964** with  $T_{ext}(Y) = [0, 0.5, 0.5]^{\top} \notin Conv(S(Y))$  and  $T_{\text{proj}}(Y) = [0.5, 0.25, 0.25]^\top \in \text{Conv}(S(Y))$ . By varying  $\delta$ , we control the projection distance  $d(T, S)$  between

<span id="page-17-2"></span>

Figure 9: Synthetic experiment. Accuracy of the global model as a function of the projection distance  $d(T, S)$  between the target distribution  $T(Y)$  and client label distributions  $Conv(S(Y))$ . Means and standard deviations reported over 5 independent runs.

**965** each  $T_\delta$  and  $Conv(S)$  from solving equation [6,](#page-4-2) allowing us to study its effect on model performance.

**966 967 968 969 970 971** We evaluate the global model on a test set with  $n_{test} = 2000$  samples drawn from the target distribution  $T(Y)$  for each value of  $\delta$  and record the target accuracy for FedPALS and FedAvg. Figure [9](#page-17-2) illustrates the relationship between the target accuracy and the projection distance  $d(T, S)$  due to varying  $\delta$ . When  $d(S, T) = 0$  (i.e.,  $T(Y) \in Conv(S)$ ), the target accuracy is highest, indicating that our method successfully matches the target distribution. As  $d(S, T)$  increases (i.e., T moves further away from  $Conv(S)$ , the task becomes harder and accuracy declines. For all values, FedPALS performs better than FedAvg. For more details on the synthetic experiment, see Appendix [A.](#page-14-0)

#### <span id="page-18-0"></span>**972 973** C PROOFS

#### **974 975** C.1 FEDPALS UPDATES

**976 977 978 979 980 981 Proposition [1](#page-3-1) (Repeated)** (Unbiased SGD update). Consider a single round  $t$  of federated learning in the batch stochastic gradient setting with learning rate  $\eta$ . Each client  $i \in [M]$  is given parameters  $\theta_t$  by the server, computes their local gradient, and returns the update  $\theta_{i,t} = \theta_t - \eta \nabla_{\theta} \hat{R}_i(h_{\theta_t})$ . Let weights  $\alpha^c$  satisfy  $T(X,Y) = \sum_{i=1}^M \alpha_i^c S_i(X,Y)$ . Then, the aggregate update  $\theta_{t+1} = \sum_{i=1}^M \alpha_i^c \theta_{i,t}$ satisfies

$$
\mathbb{E}[\theta_{t+1} | \theta_t] = \mathbb{E}[\theta_{t+1}^T | \theta_t],
$$

where  $\theta^T_{t+1}$  is the batch stochastic gradient update for  $\hat{R}_T$  that would be obtained with a sample from the target domain.

*Proof.*

$$
\theta_{t+1} = \sum_{i=1}^{M} \alpha_i^c \theta_{i,t} = \sum_{i=1}^{M} \theta_i^c (\theta_t - \eta \nabla \hat{R}_i(h_{\theta_t})) = \theta_t - \eta \sum_{i=1}^{M} \alpha_i \nabla \hat{R}_i(h_{\theta_t})
$$
(9)

$$
\begin{array}{c} 989 \\ 990 \\ 991 \end{array}
$$

> $\mathbb{E}[\theta_{t+1} \mid \theta_t] = \theta_t - \eta \cdot \mathbb{E}\left[ \sum_{i=1}^M \right]$  $i=1$  $\alpha_i \nabla \hat{R}_i(h_{\theta_t}) \mid \theta_t$ 1 (10)

$$
= \theta_t - \eta \cdot \sum_{x,y} \mathbb{E}\left[\sum_{i=1}^M \hat{S}_i(x,y)\alpha_i\right] \nabla L(y, h_{\theta_t}(x)) \tag{11}
$$

$$
= \theta_t - \eta \cdot \sum_{x,y} T(x,y) \nabla L(y, h_{\theta_t}(x)) \tag{12}
$$

$$
= \theta_t - \eta \cdot \mathbb{E}\left[\sum_{x,y} \hat{T}(x,y)\right] \nabla L(y, h_{\theta_t}(x)) = \mathbb{E}[\theta_{t+1}^T \mid \theta_t]. \tag{13}
$$

 $\Box$ 

**1001 1002 1003**

**1005**

**1007 1008 1009**

**1013 1014**

**1018**

#### **1004** C.2 FEDPALS IN THE LIMITS

**1006** As  $\lambda \to \infty$ , because the first term in equation [7](#page-4-3) is bounded, the problem shares solution with

$$
\min_{\alpha_1,\dots,\alpha_M} \sum_i \frac{\alpha_i^2}{n_i} \quad \text{s.t.} \quad \sum_i \alpha_i = 1, \quad \forall i : \alpha_i \ge 0 \,. \tag{14}
$$

**1010** Moreover, we have the following result.

**1011 1012** Proposition 3. *The optimization problem*

$$
\min_{\alpha} \sum_{i} \frac{\alpha_i^2}{n_i} \quad s.t \quad \sum_{i} \alpha_i = 1 \quad \alpha_i \ge 0 \,\forall \, i \,,
$$

**1015 1016 1017** *has the optimal solution*  $\alpha_i^* = \frac{n_i}{\sum_i n_i}$  where  $i \in [1, m]$ 

*Proof.* From the constrained optimization problem we form a Lagrangian formulation

1019  
1020  
1021  
1022  

$$
\mathcal{L}(\alpha, \mu, \tau) = \sum_{i} \frac{\alpha_i^2}{n_i} + \mu \left( 1 - \sum_{i} \alpha_i \right) + \tau \underbrace{-\alpha}_{g(\alpha)}
$$
1022

**1023 1024** We then use the KKT-theorem to find the optimal solution to the problem.

$$
\nabla_{\alpha} \mathcal{L}(\alpha^*) = 0 \implies \forall i: 2 \frac{\alpha_i^*}{n_i} - \mu - \tau = 0.
$$
 (15)

 In other words, the following ratio is a constant,

 

 

   $\forall i \quad \frac{\alpha_i^*}{\cdots}$  $\frac{a_i}{n_i} = c$ 

 for some constant c. We have the additional conditions of primal feasibility, i.e.

$$
h(\alpha^*) = 0
$$
  

$$
g(\alpha^*) \le 0
$$

 From the first constraint, we have  $\sum_{i=1}^{M} \alpha_i^* = 1$ , and thus,

$$
\sum_{i=1}^M \alpha_i^* = c \sum_{i=1}^M n_i = 1
$$

 which implies that  $c = 1/\sum_{i=1}^{M} n_i$  and thus

$$
\forall i : \alpha_i^* = \frac{n_i}{\sum_{i=1}^M n_i}.
$$

