

Personalized Federated Learning with Contextualized Generalization

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Abstract

The prevalent personalized federated learning (PFL) usually pursues a trade-off between personalization and generalization by maintaining a shared global model to guide the training process of local models. However, the sole global model may easily transfer deviated context knowledge to some local models when multiple latent contexts exist across the local datasets. In this paper, we propose a novel concept called *contextualized generalization (CG)* to provide each client with fine-grained context knowledge that can better fit the local data distributions and facilitate faster model convergence, based on which we properly design a framework of PFL, dubbed *CGPFL*. We conduct detailed theoretical analysis, in which the convergence guarantee is presented and $\mathcal{O}(\sqrt{K})$ speedup over most existing methods is granted. To quantitatively study the generalization-personalization trade-off, we introduce the ‘generalization error’ measure and prove that the proposed *CGPFL* can achieve a better trade-off than existing solutions. Moreover, our theoretical analysis further inspires a heuristic algorithm to find a near-optimal trade-off in *CGPFL*. Experimental results on multiple real-world datasets show that our approach surpasses the state-of-the-art methods on test accuracy by a significant margin.

1 Introduction

Recently, personalized federated learning (PFL) has emerged as an alternative to conventional federated learning (FL) to cope with the statistical heterogeneity of local datasets (a.k.a., Non-I.I.D. data). Different from conventional FL that focuses on training a shared global model to explore the global optima of the whole system, i.e., minimizing the averaged loss of clients, the PFL aims at developing a personalized model (distinct from the individually trained local model which usually fail to work due to the insufficient local data and the limited diversity of local dataset) for each client to properly cover diverse data distributions. To develop the personalized

model, each user needs to incorporate some context information into the local data, since the insufficient local data cannot present the complete context which the personalized model will be applied to [Kairouz *et al.*, 2019]. However, the context is generally latent and can be hardly featurized in practice, especially when the exchange of raw data is forbidden. In the existing PFLs, the latent context knowledge can be considered to be transferred to the local users via the global model update. During the PFL training, the personalization usually requires personalized models to fit local data distributions as well as possible, while the generalization needs to exploit the common context knowledge among clients by collaborative training. Thus, the PFL is indeed pursuing a trade-off between them to achieve better model accuracy than the traditional FL. More specifically, the server-side model is trained by aggregating local model updates from each client and hence can obtain the common context knowledge covering diverse data distributions. Such knowledge can then be offloaded to each client and contributes to the generalization of personalized models.

Despite the recent PFL approaches have reported better performance against conventional FL methods, they may still be constrained in personalization by using sole global model as the guidance during the training process. Concretely, our intuition is that: If there exists multiple latent contexts across local data distributions, then contextualized generalization can provide fine-grained context knowledge and further facilitate the personalized models toward better recognition accuracy and faster model convergence. We thus argue one potential bottleneck of current PFL methods is the loss of generalization diversity with only one global model. Worse still, the global model may also easily degrade the overall performance of PFL models due to negative knowledge transfers between the disjoint contexts.

In this paper, we design a novel PFL training framework, dubbed *CGPFL*, by involving the proposed concept, i.e., *contextualized generalization (CG)*, to handle the challenge of the context-level heterogeneity. More specifically, we suppose the participating clients can be covered by several latent contexts based on their statistical characteristics and each latent context can be corresponded to a generalized model maintained in the server. The personalized models are dynamically associated with the most pertinent generalized model and guided by it with fine-grained contextualized gen-

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eralization in an iterative manner. We formulate the process as a bi-level optimization problem considering both the global models with contextualized generalization maintained in the server and the personalized models trained locally in clients.

The main contributions of this work are summarized as follows:

- To the best of our knowledge, we are the first to propose the concept of *contextualized generalization (CG)* to provide fine-grained generalization and seek a better trade-off between personalization and generalization in PFL, and further formulate the training as a bi-level optimization problem that can be solved effectively by our designed *CGPFL* algorithm.
- We conduct detailed theoretical analysis to provide the convergence guarantee and prove that *CGPFL* can obtain a $\mathcal{O}(\sqrt{K})$ times acceleration over the convergence rate of most existing algorithms for non-convex and smooth case. We further derive the generalization error bound of *CGPFL* and demonstrate that the proposed *contextualized generalization* can constantly help reach a better trade-off between personalization and generalization in terms of generalization error against the state-of-the-arts works.
- We provide a heuristic improvement of *CGPFL*, dubbed *CGPFL-Heur*, by minimizing the generalization bound in the theoretical analysis, to find a near-optimal trade-off between personalization and generalization. *CGPFL-Heur* can achieve a near-optimal accuracy with negligible additional computation in the server, while retaining the same convergence rate as that of *CGPFL*.
- Experimental results on multiple real-world datasets demonstrate that our proposed methods, i.e., *CGPFL* and *CGPFL-Heur*, can achieve higher model accuracy than the state-of-the-art PFL methods in both convex and non-convex cases.

2 Related Work

Considering that one shared global model can hardly fit the heterogeneous data distributions, some recent FL works [Ghosh *et al.*, 2020; Sattler *et al.*, 2020; Briggs *et al.*, 2020; Mansour *et al.*, 2020] try to cluster the participating clients into multiple groups and develop corresponding number of shared global models by aggregating the local updates. After the training process, the obtained global models are offloaded to the corresponding clients for inference. Since these methods only reduce the FL training into several sub-groups, of which each global model is still shared by their in-group clients, the personalization is scarce and the offloaded models can still hardly cover the heterogeneous data distributions across the in-group clients. Specifically, *IFCA* [Ghosh *et al.*, 2020] requires each client to calculate the losses on all global models to estimate its cluster identity during each iteration, and result in significantly higher computation cost. *CFL* [Sattler *et al.*, 2020] demonstrates that the conventional FL even cannot converge in some Non-I.I.D. settings and provides intriguing perspective for clustered FL with bi-partitioning clustering. However, it can only work for

some special Non-I.I.D. case described as ‘*same feature & different labels*’ [Hsieh *et al.*, 2020]. *FL+HC* [Briggs *et al.*, 2020] divides the clients clustering and the model training processes separately, and only conducts the clustering once at a manually defined step, while the training remains the same as conventional FL. Last, three effective PFL approaches are proposed in [Mansour *et al.*, 2020], of which the user clustering method is very similar to *IFCA* [Ghosh *et al.*, 2020].

Most recently, the PFL approaches have attracted increasing attention [Kairouz *et al.*, 2019]. Among them, a branch of works [Hanzely and Richtárik, 2020; Hanzely *et al.*, 2020; Deng *et al.*, 2020] propose to mix the global model on the server with local models to acquire the personalized models. More concretely, Hanzely *et al.* [Hanzely *et al.*, 2020; Hanzely and Richtárik, 2020] formulate the mixture problem as a combined optimization of the local and global models, while *APFL* [Deng *et al.*, 2020] straightforwardly mixes them with an adaptive weight. *KT-pFL* [Zhang *et al.*, 2021] exploits the knowledge distillation (KD) to transfer the generalization information to local models and allows the training of heterogeneous models in FL setting. Differently, *FedPer* [Arivazhagan *et al.*, 2019] splits the personalized models into two separate parts, of which the base layers are shared by all the clients and trained on the server, and the personalization layers are trained to adapt to individual data and maintain the privacy properties on local devices. *MOCHA* [Smith *et al.*, 2017] considers the model training on the clients as relevant tasks and formulate this problem as a distributed multi-task learning objective. Fallah *et al.* [Fallah *et al.*, 2020] make use of the model agnostic meta learning (*MAML*) to implement the PFL, of which the obtained meta-model contains the generalization information and can be utilized as a good initialization point of training.

3 Problem Formulation

We start by formalizing the FL task and then introduce our proposed method. Given N clients and their Non-I.I.D. datasets $\tilde{D}_1, \dots, \tilde{D}_i, \dots, \tilde{D}_N$ that subject to the underlying distributions as $D_1, \dots, D_i, \dots, D_N$ ($D_i \in \mathbb{R}^{d \times n_i}$ and $i \in [N]$). Every client i has m_i instances $z^{i,j} = (\mathbf{x}^{i,j}, y^{i,j})$, $j \in [m_i]$, where \mathbf{x} is the data features and y denotes the label. Hence, the objective function of the conventional FL can be described as [Li *et al.*, 2021]:

$$\min_{\omega \in \mathbb{R}^d} \{G(\omega) := G(f_1(\omega; \tilde{D}_1), \dots, f_N(\omega; \tilde{D}_N))\}, \quad (1)$$

where ω is the global model and $f_i : \mathbb{R}^d \rightarrow \mathbb{R}$, $i \in [N]$ denotes the expected loss function over the data distribution of client i : $f_i(\omega; \tilde{D}_i) = \mathbb{E}_{z^{i,j} \in \tilde{D}_i} [f_i(\omega; z^{i,j})]$. The function $G(\cdot)$ denotes the aggregation method to obtain the global model ω . For example, *FedAvg* [McMahan *et al.*, 2017] applies $G(\omega) = \sum_{i=1}^N \frac{m_i}{m} f_i(\omega)$ to do the aggregation, where m is the total number of instances on local devices.

To handle the challenge of rich statistical diversities in PFL, especially in the cases where the local datasets belong to several latent contexts, our *CGPFL* propose to maintain K context-level generalized models in the server to guide the training of personalized models on the clients. During training, the local training process based on its local dataset can

push the personalized model to fit its local data distribution as well as possible. Meanwhile, the regularizer will dynamically *pull* the personalized model as close as possible to the most pertinent generalized model during the iterative algorithm, from which the fine-grained context knowledge can be transferred to each personalized model to better balance the generalization and personalization. Hence, the overall objective function of *CGPFL* can be described as a bi-level optimization problem as:

$$\begin{aligned} \min_{\Theta \in \mathbb{R}^{d \times N}} \frac{1}{N} \sum_{i=1}^N \left\{ F_i(\theta_i) := f_i(\theta_i) + \lambda r(\theta_i, \omega_k^*) \right\}, i \in C_k^*, \\ \text{s.t. } \Omega^*, C_K^* = \arg \min_{\Omega \in \mathbb{R}^{d \times K}, C_K} G(\omega_1, \dots, \omega_K; C_K), \end{aligned}$$

where θ_i ($i \in [N]$) denotes the personalized model on client i and $\Theta = [\theta_1, \dots, \theta_N]$. The context-level generalized models are denoted by $\Omega = [\omega_1, \dots, \omega_K]$. λ is a hyper-parameter and C_k denotes the corresponding context that client i belongs to. Considering the latent contexts are represented in disjoint subspaces respectively, the function $G(\cdot)$ can be decomposed as $G(\omega_1, \dots, \omega_K; C_K) = \frac{1}{K} \sum_{k=1}^K G_k(\omega_k; C_k)$.

In general, there exists two alternative strategies to generate the context-level generalized models. The intuitive one is to solve the inner-level objective $\min_{\Omega \in \mathbb{R}^{d \times K}} G(\omega_1, \dots, \omega_K)$ based on local datasets, which is similar to *IFCA* [Ghosh *et al.*, 2020]. However, the computation overhead is high in the local devices while their available computation resources are usually limited. Comparing the local objective that trains a generalized model ω_k based on local dataset, i.e., $\omega_k^* = \arg \min_{\omega} f_i(\omega; \tilde{D}_i)$, with that of the personalized model,

i.e., $\theta_i^* = \arg \min_{\theta_i} \{f_i(\theta_i; \tilde{D}_i) + \lambda r(\theta_i, \omega_k^*)\}$, we notice that

the locally obtained θ_i^* can be regarded as the distributed estimation of ω_k^* . In this way, the regularizer $r(\theta_i^*, \omega_k^*)$ can be used to evaluate the estimation error, and we can further derive the context-level generalized models by minimizing the average estimation error. In this paper, we use L_2 -norm i.e., $r(\theta_i, \omega_k) = \frac{1}{2} \|\theta_i - \omega_k\|^2$ as the regularizer, which is also adopted in various prevalent PFL methods [Hanzely and Richtárik, 2020; Hanzely *et al.*, 2020; T Dinh *et al.*, 2020; Li *et al.*, 2021] and has been empirically demonstrated to be superior over other regularizers, e.g., the symmetrized KL divergence in [Li *et al.*, 2021]. Hence, we formulate our overall objective as:

$$\begin{aligned} \min_{\Theta \in \mathbb{R}^{d \times N}} \frac{1}{N} \sum_{i=1}^N \left\{ F_i(\theta_i) := f_i(\theta_i) + \frac{\lambda}{2} \|\theta_i - \omega_k^*\|^2 \right\}, i \in C_k^*, \\ \text{s.t. } \Omega^*, C_K^* = \arg \min_{\Omega \in \mathbb{R}^{d \times K}, C_K} \sum_{k=1}^K q_k \sum_{j \in C_k} p_{k,j} \|\theta_j - \omega_k\|^2, \quad (2) \end{aligned}$$

We adopt $p_{k,j} = \frac{1}{|C_j|}$ and $q_k = \frac{|C_k|}{N}$ in this paper, where C_k ($k \in [K]$) denotes the latent context k , and $|C_k|$ is the number of clients that belong to the context k . Intriguingly, the inner-level objective is exactly the classic objective of k -means clustering [Lloyd, 1982]. We notice that when $K = 1$, the above objective is equivalent to the overall objective in [T Dinh *et al.*, 2020], which means that the objective in [T Dinh *et al.*, 2020] can be regarded as a *special case* ($K = 1$) of ours.

4 Design of *CGPFL*

In this section, we introduce our proposed *CGPFL* in detail. The key idea is to dynamically relate the clients to K latent contexts based on their uploaded local model updates, and then develop a generalized model for each context by aggregating the updates from each user group. These generalized models are utilized to guide the training directions of personalized models and transfer contextualized generalization to them. Both the personalized models and the generalized models are trained in parallel, so we can denote the model parameters in matrix form. The generalized models can be written as $\Omega_K := [\omega_1, \dots, \omega_k, \dots, \omega_K] \in \mathbb{R}^{d \times K}$, and the corresponding local approximations are $\Omega_{I,R} := [\tilde{\omega}_{1,R}, \dots, \tilde{\omega}_{i,R}, \dots, \tilde{\omega}_{N,R}]$, where R is the number of local iterations and $\tilde{\omega}_{i,R}, \omega_k \in \mathbb{R}^d, \forall i \in [N], k \in [K]$. In this paper, we use capital characters to represent matrices unless stated otherwise.

4.1 *CGPFL*: Algorithm

We design an effective alternating optimization framework to minimize the overall objective in (2). Specifically, the upper-level problem can be decomposed into N separate sub-problems with fixed generalized models and to be solved on local devices in parallel. Next, we can further settle the inner-level problem to derive the generalized models with fixed personalized models. Since the solution to the sub-problems of the upper-level objective has been well-explored in recent PFL methods [T Dinh *et al.*, 2020; Li *et al.*, 2021; Hanzely *et al.*, 2020], we hereby mainly focus on the inner-level problem. We alternately update the context-level generalized models Ω_K and the context indicator C_K to obtain the optimal generalized models. We view the personalized models, i.e., $\Theta_I = [\theta_i, \dots, \theta_N]$, as private data, and distributionally update the context-level generalized models Ω_K on clients with fixed context indicator C_K . During each server round, the server conducts k -means clustering on uploaded local parameters $\Omega_{I,R}^t$ to cluster the clients into K latent contexts, and the clustering results C_K are re-arranged to the matrix form as $P^t \in \mathbb{R}^{N \times K}$. For example, if client $i, i \in [N]$ is clustered into the context $C_j, j \in [K]$ (where $C_j, j \in [K]$ are sets, the union $\bigcup_{j \in [K]} C_j$ and intersection $\bigcap_{j \in [K]} C_j$ are the set $[N]$ and empty set, respectively), the element $(P^t)_{i,j}$ is defined as $\frac{1}{|C_j|}$, or set 0 otherwise. In this way, the elements of every column in P^t amount to 1, i.e. $\sum_{i=1}^N (P^t)_{i,j} = 1, \forall j, t$.

When considering the relationship between the consecutive P^t , we can formulate the iterate as $P^{t+1} = P^t Q^t$, where $Q^t \in \mathbb{R}^{K \times K}$ is a square matrix. We can find that to maintain the above property of P^t ($\forall t$), the matrix Q^t must satisfies that:

$$\sum_{j=1}^K (Q^t)_{j,k} = 1, \forall k, t \quad \text{and} \quad \sum_{k=1}^K (Q^t)_{j,k} = 1, \forall j, t. \quad (3)$$

It is noticed that the clustering is based on the latest model parameters Ω_I^{t+1} that depends on Ω_I^t , and the latest gradient updates given by clients. Hence, P^{t+1} is determined by and only by P^t and Q^t . Then we can consider this global iteration as a discrete-time Markov chain and Q^t corresponds the transition probability matrix.

Algorithm 1 *CGPFL*: Personalized Federated Learning with Contextualized Generalization

Input: $\Theta_I^0, \Omega_K^0, P^0, T, R, S, K, \lambda, \eta, \alpha, \beta$.

Output: Θ_I^T .

```

1: for  $t = 0$  to  $T - 1$  do
2:   Server sends  $\Omega_K^t$  to clients according to  $P^t$ .
3:   for local device  $i = 1$  to  $N$  in parallel do
4:     Initialization:  $\Omega_{I,0}^t = \Omega_K^t J^t$ .
5:     Local update for the sub-problem of  $G(\Theta_I, \Omega_K)$ :
6:     for  $r = 0$  to  $R - 1$  do
7:       for  $s = 0$  to  $S - 1$  do
8:         Update personalized model:  $\theta_i^{s+1} = \theta_i^s - \eta \nabla F_i(\theta_i^s)$ .
9:       end for
10:      Local update:  $\tilde{\omega}_{i,r+1}^t = \tilde{\omega}_{i,r}^t - \beta \nabla_{\omega_i} G(\tilde{\theta}_i(\tilde{\omega}_{i,r}^t), \tilde{\omega}_{i,r}^t)$ .
11:    end for
12:  end for
13:  Clients send back  $\tilde{\omega}_{i,R}^t$  and server conducts clustering (e.g.,
     $k$ -means++) on models  $\Omega_{I,R}^t$  to obtain  $P^{t+1}$ .
14:  Global aggregation:  $\Omega_K^{t+1} = \Omega_K^t - \alpha(\Omega_K^t - \Omega_{I,R}^t P^{t+1})$ .
15: end for
16: return The personalized models  $\Theta_I^T$ .
```

During each local round, the clients need to first utilize local datasets to solve the regularized optimization objective, i.e., the upper-level objective in (2) with fixed $\tilde{\omega}_{i,r}^t$ to obtain a δ -approximate solution $\tilde{\theta}_i(\tilde{\omega}_{i,r}^t)$. Then, each client is required to calculate the gradients $\nabla_{\omega_i} G(\tilde{\theta}_i(\tilde{\omega}_{i,r}^t), \tilde{\omega}_{i,r}^t)$ with fixed $\tilde{\theta}_i(\tilde{\omega}_{i,r}^t)$ and update the model using $\tilde{\omega}_{i,r+1}^t = \tilde{\omega}_{i,r}^t - \beta \nabla_{\omega_i} G(\tilde{\theta}_i(\tilde{\omega}_{i,r}^t), \tilde{\omega}_{i,r}^t)$, where β is the learning rate and $\nabla_{\omega_i} G(\tilde{\theta}_i(\tilde{\omega}_{i,r}^t), \tilde{\omega}_{i,r}^t) = \frac{2}{N} \nabla r(\tilde{\theta}_i(\tilde{\omega}_{i,r}^t), \tilde{\omega}_{i,r}^t)$. To reduce the communication overhead, our *CGPFL* allows the clients to process several local iterations before uploading the latest model parameters to the server. The details of *CGPFL* is given in algorithm 1, from which we can summarize the parameters update process as:

$$\Omega_{I,R}^{t-1} \xrightarrow{P^t} \Omega_K^t \xrightarrow{J^t} \Omega_{I,0}^t \xrightarrow{H_I^t} \Omega_{I,R}^t \xrightarrow{P^{t+1}} \Omega_K^{t+1}, \quad (4)$$

where $P^{t+1} = P^t Q^t$ and $J^t P^t = I_K$ ($J^t \in \mathbb{R}^{K \times N}$ and I_K is an identity matrix), $\forall t$.

4.2 Convergence Analysis

Since the inner-level objective in (2) is non-convex, we focus on analyzing the convergence rate under the smooth case. Firstly, we can write the local updates as:

$$\Omega_{I,R}^t = \Omega_{I,0}^t - \beta R H_I^t, \quad (5)$$

where $H_I^t = \frac{1}{R} \sum_{r=0}^{R-1} H_{I,r}^t$ and $H_{I,r}^t = \frac{2}{N} (\Omega_{I,r}^t - \tilde{\Theta}_I(\Omega_{I,r}^t))$. Based on (5) and the update process in (4), we can obtain the global updates as:

$$\begin{aligned} \Omega_K^{t+1} &= (1 - \alpha) \Omega_K^t + \alpha \Omega_{I,R}^t P^{t+1} \\ &= \Omega_K^t [(1 - \alpha) I_K + \alpha Q^t] - \alpha \beta R H_I^t P^t Q^t. \end{aligned}$$

Definition 1 (*L-smooth*) (i.e., *L-Lipschitz gradient*) If a function f satisfies $\|\nabla f(\omega) - \nabla f(\omega')\| \leq L \|\omega - \omega'\|$, $\forall \omega, \omega'$, we say f is *L-smooth*.

Assumption 1 (Smoothness) The loss functions f_i is *L-smooth* and $G(\omega_k)$ is *L_G-smooth*, $\forall i, k$.

Assumption 2 (Bounded intra-context diversity) The variance of local gradients to the corresponding context-level generalized models is upper bounded by:

$$\frac{1}{|C_k|} \sum_{i \in C_k} \|\nabla G_{k,i}(\omega_k) - \nabla G_k(\omega_k)\|^2 \leq \delta_G^2, \forall k \in [K], \quad (6)$$

where $G_{k,i}(\omega_k) := r(\theta_i, \omega_k)$.

Assumption 3 (Bounded parameters and gradients) The generalized model parameters Ω_K^t and the gradients $\nabla G_K(\Omega_K^t)$ are upper bounded by ρ_Ω and ρ_g , respectively.

$$\|\Omega_K^t\|^2 \leq \rho_\Omega^2 \quad \text{and} \quad \|\nabla G_K(\Omega_K^t)\|^2 \leq \rho_g^2, \quad \forall t \quad (7)$$

where ρ_Ω and ρ_g are finite non-negative constants, and $\nabla G_K(\Omega_K^t) := [\nabla G_1(\omega_1^t), \dots, \nabla G_k(\omega_k^t), \dots, \nabla G_K(\omega_K^t)]$.

Proposition 1 [T Dinh et al., 2020] The deviation between the δ -approximate and the optimal solution is upper bounded by δ . That is:

$$\mathbb{E} \left[\|\tilde{\Theta}_I(\Omega_{I,r}^t) - \hat{\Theta}_I(\Omega_{I,r}^t)\|^2 \right] \leq N \delta^2, \forall r, t, \quad (8)$$

where $\tilde{\Theta}_I$ is the δ -approximate solution and $\hat{\Theta}_I$ is the matching optimal solution.

Assumption 1 provides typical conditions for convergence analysis, and assumption 2 is common in analyzing algorithms that are built on SGD. As for assumption 3, the model parameters are easily bounded by using projection during the model training process, while the gradients can be bounded with the smooth condition and bounded model parameters. To evaluate the convergence of the proposed *CGPFL*, we adopt the technique used in [T Dinh et al., 2020] to define that:

$$\mathbb{E} \left[\frac{1}{K} \|\nabla G_K(\Omega_K^{t*})\|^2 \right] := \frac{1}{T} \sum_{t=0}^{T-1} \mathbb{E} \left[\frac{1}{K} \|\nabla G_K(\Omega_K^t)\|^2 \right],$$

where t^* is uniformly sampled from the set $\{0, 1, \dots, T-1\}$.

Theorem 4.1 (Convergence of *CGPFL*) Suppose Assumption 1, 2 and 3 hold. If $\beta \leq \frac{1}{2\sqrt{R(R+1)L_G^2}}$, $\forall R \geq 1$, $\alpha \leq 1$,

and $\hat{\alpha}_0 := \min \left\{ \frac{8\alpha^2 \rho_\Omega^2}{K \Delta_G}, \sqrt{\frac{4}{3}} \frac{\alpha \rho_\Omega}{\rho_g}, \sqrt{\frac{1}{416 L_G^2}} \alpha \right\}$, where Δ_G is

defined as $\Delta_G := \mathbb{E} \left[\frac{1}{K} \sum_{k=1}^K G_k(\omega_k^0) - \frac{1}{K} \sum_{k=1}^K G_k(\omega_k^T) \right]$,

we have:

- The convergence of the generalized models:

$$\begin{aligned} & \frac{1}{K} \mathbb{E} \left[\|\nabla G_K(\Omega_K^{t*})\|^2 \right] \\ & \leq \mathcal{O} \left(\frac{48\alpha^2 (\rho_\Omega^2/K)}{\hat{\alpha}_0^2 T} + \frac{80(26(\rho_\Omega^2/K)L_G^2 \delta^2)^{\frac{1}{2}}}{\sqrt{NKR T}} + \frac{52\delta^2}{KN} \right). \end{aligned}$$

- The convergence of the personalized models:

$$\begin{aligned} & \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\|\tilde{\Theta}_I^{t*} - \Omega_K^{t*} J^{t*}\|^2 \right] \\ & \leq \mathcal{O} \left(\frac{1}{K} \mathbb{E} \left[\|\nabla G_K(\Omega_K^{t*})\|^2 \right] \right) + \mathcal{O} \left(\frac{\delta_G^2}{\lambda^2} + \delta^2 \right). \end{aligned}$$

Remark 4.1 Theorem 4.1 shows that the proposed *CGPFL* can achieve a convergence rate of $\mathcal{O}(1/\sqrt{KNRT})$, which is $\mathcal{O}(\sqrt{K})$ times faster than what most of the state-of-the-art works [Karimireddy et al., 2020; Deng et al., 2020; Reddi et al., 2020] achieved (i.e., $\mathcal{O}(1/\sqrt{NRT})$) in non-convex FL setting. The detailed proof of convergence can be found in the full version of this paper [Tang et al., 2021].

4.3 Generalization Error

We analyse the generalization error of *CGPFL* in this section. Before starting the analysis, we first introduce two important definitions as follows.

Definition 2 (Complexity) *Let \mathcal{H} be a hypothesis class (corresponding to $\omega \in \mathbb{R}^d$ in neural network), and $|D|$ be the size of dataset D , the complexity of \mathcal{H} can be expressed by the maximum disagreement between two hypotheses on the dataset D :*

$$\lambda_{\mathcal{H}}(D) = \sup_{h_1, h_2 \in \mathcal{H}} \frac{1}{|D|} \sum_{(x,y) \in D} |h_1(x) - h_2(x)|. \quad (9)$$

Definition 3 (Label-discrepancy) *Consider a hypothesis class \mathcal{H} , the label-discrepancy between two data distributions D_1 and D_2 is given by:*

$$\text{disc}_{\mathcal{H}}(D_1, D_2) = \sup_{h \in \mathcal{H}} |\mathcal{L}_{D_1}(h) - \mathcal{L}_{D_2}(h)|, \quad (10)$$

where $\mathcal{L}_D(h) = \mathbb{E}_{(x,y) \in D} [l(h(x), y)]$.

Theorem 4.2 (Generalization error bound of *CGPFL*) *When Assumption 1 is satisfied, with probability at least $1 - \delta$, the following holds:*

$$\begin{aligned} & \sum_{i=1}^N \frac{m_i}{m} \left\{ \mathcal{L}_{D_i}(\hat{h}_i^*) - \min_{h \in \mathcal{H}} \mathcal{L}_{D_i}(h) \right\} \\ & \leq 2\sqrt{\frac{\log \frac{N}{\delta}}{m}} + \sqrt{\frac{dK}{m} \log \frac{em}{d}} + \left(\lambda + \frac{L}{2}\right) \text{cost}(\Theta^*, \Omega^*; K) \\ & + \sum_{i=1}^N \frac{m_i}{m} \left\{ 2B \lambda_{\mathcal{H}}(D_i) + \text{disc}(D_i, \tilde{D}_i) \right\}, \end{aligned}$$

where B is a positive constant with $|\mathcal{L}_D(h_1) - \mathcal{L}_D(h_2)| \leq B \lambda_{\mathcal{H}}(D)$, $\forall h_1, h_2 \in \mathcal{H}$. Besides, \hat{h}_i^* is given by $\hat{h}_i^* = \arg \min_{\theta_i} \left\{ \mathcal{L}_{\tilde{D}_i}(h(\theta_i)) + \|\theta_i - \omega_k^*\|^2 \right\}$ and $\text{cost}(\Theta^*, \Omega^*; K) = \sum_{i=1}^N \frac{m_i}{m} \min_{k \in [K]} \|\theta_i^* - \omega_k^*\|^2$.

Remark 4.2 Theorem 4.2 gives the generalization error bound of *CGPFL*. When $K = 1$, it yields the error bound of PFL with single global model [Li *et al.*, 2021; T Dinh *et al.*, 2020; Hanzely and Richtárik, 2020; Hanzely *et al.*, 2020]. As the number of contexts increases, the second terms become larger, while the last term get smaller. Hence, our *CGPFL* can always reach better personalization-generalization trade-off by adjusting the number of contexts K , and further achieve higher accuracy than the existing PFL methods. The detailed proof of generalization error can be found in the full version of this paper [Tang *et al.*, 2021].

4.4 *CGPFL-Heur*: The Heuristic Improvement

As discussed, Theorem 4.2 indicates that there exists an optimal K^* ($K^* \in [K]$) to achieve the minimal generalization error bound that corresponds to the highest model accuracy. Theoretically, the optimal K^* can be obtained by minimizing the generalization bound in Theorem 4.2. We can find that the first and the third term have no relationship with the number of latent contexts, that is, they are irrelevant to K . Therefore, we can obtain an optimal K^* by minimizing the following expression:

$$e(K) := \sqrt{\frac{dK}{m} \log \frac{em}{d}} + \mu \cdot \text{cost}(\Theta^*, \Omega^*; K), \quad (11)$$

where μ is a hyper-parameter which is induced by the unknown constant L . The above objective can be solved in the server along with the clustering. In the down-to-earth experiments, we notice that the latent context structure can be learned efficiently in the first few rounds. Based on this observation, we believe that *CGPFL-Heur* can efficiently figure out a near-optimal solution \hat{K} by operating the solver of (11) only in the first few rounds (in the experimental part, we only operate the solver at the first global round), and after that, the obtained \hat{K} will no longer be updated. In this way, *CGPFL-Heur* can reach a near-optimal trade-off between generalization and personalization with negligible additional computation in the server. Moreover, in view of the fact that we only need to operate the solver in the first few rounds, *CGPFL-Heur* can retain the same convergence rate as *CGPFL*.

5 Experiments

5.1 Experimental Setup

Dataset Setup: Three datasets including MNIST [LeCun *et al.*, 1998], CIFAR10 [Krizhevsky, 2009], and Fashion-MNIST (FMNIST) [Xiao *et al.*, 2017] are used in our experiments. To generate Non-I.I.D. datasets for the clients, we split the whole dataset as follows. 1) MNIST: we distribute the train-set containing 60,000 digital instances into 40 clients, and each of them is only provided with 3 classes out of total 10. The number of instances obtained by each client is randomly chosen from the range of [400, 5000], of which 75% are used for training and the remaining 25% for testing. 2) CIFAR10: We distribute the whole dataset containing 60,000 instances into 40 clients, and each of them is also provided with 3 classes out of total 10. The number of instances obtained by each client is randomly chosen from the range of [400, 5000]. The train/test split remains 75%/25%. 3) Fashion-MNIST: It's a more challenging replacement of MNIST, and the Non-I.I.D. splitting is the same as MNIST.

Competitors: We compare our *CGPFL* and *CGPFL-Heur* with seven state-of-the-art works: one traditional FL method, *FedAvg* [McMahan *et al.*, 2017]; one typical cluster-based FL method, *IFCA* [Ghosh *et al.*, 2020]; and five most recent PFL models, *APFL* [Deng *et al.*, 2020], *Per-FedAvg* [Falah *et al.*, 2020], *L2SGD* [Hanzely and Richtárik, 2020], *pFedMe* [T Dinh *et al.*, 2020], and *Ditto* [Li *et al.*, 2021].

Model Architectures: 1) For strongly convex case, we use a l_2 -regularized multinomial logistic regression model (MLR) with the softmax and cross-entropy loss, in line with [T Dinh *et al.*, 2020]; 2) For the non-convex case, we apply a neural network (DNN) with one hidden layer of size 128 and a softmax layer at the end for evaluation. In addition, we apply a CNN that has two convolutional layers and two fully connected layers for the CIFAR10. All competitors and our algorithms are based on the same configurations and fine-tuned to their best performances.

5.2 Overall Performance

The comprehensive comparison results of our *CGPFL* and *CGPFL-Heur* are shown in Table 1. It can be observed that our methods outperform the competitors with large margins

Method	MNIST		FMNIST		CIFAR10
	MLR	DNN	MLR	DNN	CNN
<i>FedAvg</i>	88.63	91.05	82.44	83.45	46.34
<i>IFCA</i> ($K = 4$)	95.27	96.19	91.55	92.56	60.22
<i>L2SGD</i>	89.46	92.48	88.59	90.64	58.68
<i>APFL</i>	92.69	95.59	92.60	93.76	72.12
<i>pFedMe (PM)</i>	91.90	92.20	85.49	86.87	68.88
<i>Per-FedAvg (HF)</i>	92.44	93.54	87.17	87.57	71.46
<i>Ditto</i>	89.96	92.85	88.62	90.56	69.56
<i>CGPFL</i> ($K = 4$)	95.65	96.55	92.65	93.56	72.78
<i>CGPFL-Heur</i>	97.41	98.03	95.18	96.00	74.75

Table 1: Comparison of test accuracy. We set $N = 40$, $\alpha = 1$, $\lambda = 12$, $S = 5$, $lr = 0.005$ and $T = 200$ for MNIST and Fashion-MNIST (FMNIST), and $T = 300$, $lr = 0.03$ for CIFAR10, where lr denotes the learning rate.

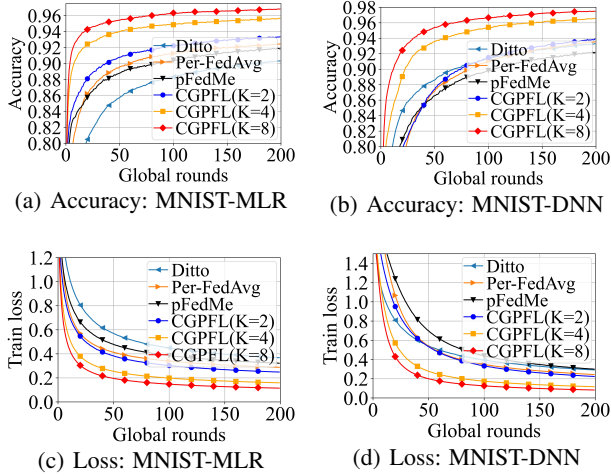


Figure 1: Performance on MNIST for different K with $N = 40$, $\alpha = 1$, $\lambda = 12$, $R = 10$, and $S = 5$.

for both non-convex and convex cases on all datasets, even if *IFCA* works with a good initialization. Besides, although we only provide the proof of convergence rate under non-convex case, as shown in Figure 1 and Figure 2, the extensive experiments further demonstrate that our methods constantly obtain better performance against multiple state-of-the-art PFL methods (*pFedMe*, *Ditto*, and *Per-FedAvg*) with faster convergence rate under both strongly-convex and non-convex cases. Specifically, the figures in Figure 1 show the results for MNIST dataset on MLR and DNN model, while the figures in Figure 2 give the results for Fashion-MNIST dataset on MLR and DNN model.

5.3 Further Evaluations on *CGPFL-Heur*

To further evaluate the performance of *CGPFL-Heur*, on the one hand, we conduct the *CGPFL* training with different number of contexts (i.e., K) varying from 1 to $N/2$ on MNIST and FMNIST, respectively. In particular, we set the maximal value of K no more than $N/2$ to avoid overfitting. By collating the model accuracy with different K , we can find out the optimal K which corresponds to the optimal personalization-generalization trade-off in *CGPFL*. The

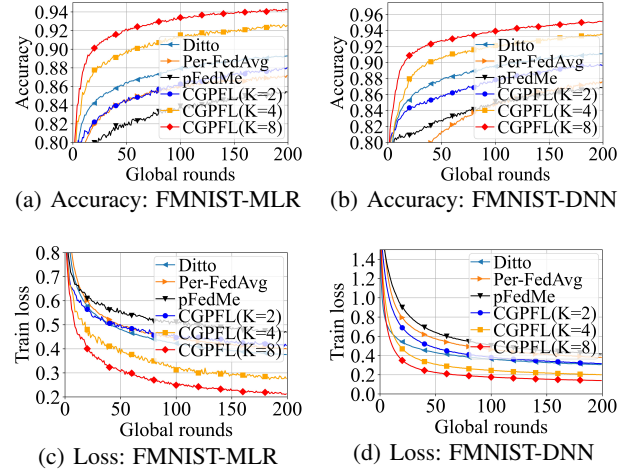


Figure 2: Performance on FMNIST for different K with $N = 40$, $\alpha = 1$, $\lambda = 12$, $R = 10$, and $S = 5$.

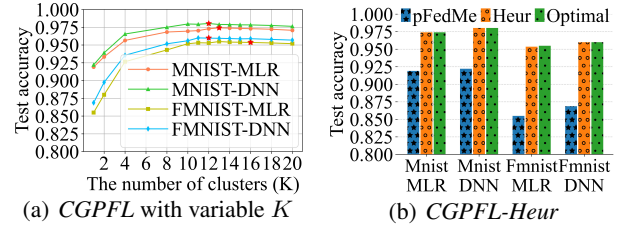


Figure 3: Further evaluations on the *CGPFL-Heur* against *CGPFL*

results are demonstrated in Figure 3(a). On the other hand, we conduct the *CGPFL-Heur* training with an appropriate μ and keep other parameters same as that of the above evaluation. As shown in Figure 3(a), we distinguish the results of *CGPFL-Heur* using red-star points. Besides, we make comparisons between the performance of a state-of-the-art PFL algorithm, *pFedMe* [T Dinh *et al.*, 2020] with our proposed *CGPFL* with optimal K and *CGPFL-Heur* in Figure 3(b). The results in Figure 3(a) and Figure 3(b) demonstrate that our designed heuristic algorithm *CGPFL-Heur* can effectively reach a near-optimal trade-off and consequently achieve the near-optimal model accuracy.

6 Conclusion

In this paper, we propose a novel personalized federated learning framework to handle the challenge of statistical heterogeneity (Non-I.I.D), especially contextual heterogeneity in the federated setting. To the best of our knowledge, we are the first to propose the concept of contextualized generalization (CG) for personalized federated learning and further formulate it to a bi-level optimization problem that is solved effectively. Our method provides fine-grained generalization knowledge for personalized models which can prompt higher test accuracy and facilitate faster model convergence. Experimental results on real-world datasets demonstrate the effectiveness of our method over the state-of-the-art works.

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