A Unified Framework for Proximal Methods

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Paper under double-blind review

ABSTRACT

We study the training of regularized neural networks where the regularizer can be non-smooth and non-convex. We propose a unified framework for stochastic proximal gradient descent, which we term PROXGEN, that allows for arbitrary positive preconditioners and lower semi-continuous regularizers. Our framework naturally encompasses standard stochastic proximal gradient methods without preconditioners as special cases. We present two important instances stemming from our approach: (i) the first proximal version of ADAM, one of the most popular adaptive SGD algorithm, and (ii) a revised version of PROXQUANT [Bai et al, 2019] that improves upon the original approach for quantization-specific regularizers by incorporating the effect of preconditioners when computing proximal mapping. We analyze the convergence of PROXGEN and show that the whole framework enjoys the same convergence rate as stochastic proximal gradient descent without preconditioners. We also empirically show the superiority of proximal methods compared to subgradient-based approaches via extensive experiments. Interestingly, our results indicate that proximal methods with non-convex regularizers are more effective than those with convex regularizers.

1 Introduction

We study the regularized training of neural networks, which can be formulated as the following (stochastic) optimization problem $f(\theta)$

oblem
$$\underbrace{\min_{\theta \in \Omega} F(\theta) := \underbrace{\mathbb{E}_{\xi \sim \mathbb{P}}[f(\theta; \xi)]}_{f(\theta; \xi)} + \mathcal{R}(\theta)$$
 (1)

where $\theta \in \mathbb{R}^p$ represents the network parameter, ξ is the random variable representing mini-batch data samples, and $\mathcal{R}(\cdot)$ is a regularizer encouraging low-dimensional structural constraints on θ .

For the *unregularized* case, i.e., when $\mathcal{R}(\theta) = 0$, stochastic gradient descent (SGD) has been a prevalent approach to solve the optimization problem stated in Eq. (1). At each iteration, SGD evaluates the gradient only on a randomly chosen subset of training samples (mini-batch). Vanilla SGD employs a uniform learning rate for all coordinates, and several adaptive variants have been proposed, which scale the learning rate for each coordinate by its gradient history. A prime example of such approaches is ADAGRAD (Duchi et al., 2011), which adjusts the learning rate by the sum of all the past squared gradients. However, the performance of ADAGRAD degrades in non-convex dense settings as the learning rates vanish too rapidly. To resolve this issue, exponential moving average (EMA) approaches such as RMSPROP (Tieleman & Hinton, 2012) and ADAM (Kingma & Ba, 2015) have been proposed and become popular. These scale down the gradients by square roots of exponential moving averages of squared past gradients to essentially limit the scope of the adaptation to only a few recent gradients. In terms of theory, convergence analyses of these unregularized SGD, whether adaptive or not, have been well studied both for convex (Kingma & Ba, 2015; Reddi et al., 2018) and non-convex (Chen et al., 2019b; Lei et al., 2019) loss f cases.

The technique of regularization is ubiquitous in machine learning as it can effectively prevent overfitting and yield better generalization. The ℓ_1 -regularized training for Lasso estimators/sparse Gaussian graphical model (GMRF) estimation (Tibshirani, 1996; Ravikumar et al., 2011) and ℓ_2 weight decay (Tychonoff, 1943) on parameters are prototypical examples. In the context of deep

Table 1. Comparison among stochastic (or online) 1 GD for solving the problem in Eq. (1).							
Algorithm	Non-convex Loss	Non-convex Regularizer	Preconditioner	Momentum	Convergence Guarantee		
ADAGRAD (Duchi et al., 2011)			ADAGRAD		✓		
Ghadimi et al. (2016)	/		1		1		
Wang et al. (2018)	<i>\</i>			1	1		
Pham et al. (2019)	/			1	1		
Davis & Drusvyatskiy (2019)	<i>\</i>			1	1		
Xu et al. (2019a)	<i>\</i>	1			1		
Xu et al. (2019b)	<i>\</i>	1	AdaGrad		1		
Prox-SGD (Yang et al., 2020)	/		✓	1			
Davis et al. (2020)	∥ ✓	✓		✓	✓		
PROXGEN (Ours)	🗸	√	/	✓	/		

Table 1: Comparison among *stochastic* (or *online*) PGD for solving the problem in Eq. (1).

learning, important instances include network pruning (Wen et al., 2016; Louizos et al., 2018), which induces a sparse network structure, and network quantization (Yang et al., 2019; Courbariaux et al., 2015; Bai et al., 2019), which gives hard constraints so that parameters have only discrete values.

In many cases, the regularizer is non-smooth around some region (Consider ℓ_1 norm at zero). Therefore, instead of using the gradient, one employs the subgradient of the objective function $F(\theta)$ in Eq. (1). Such a strategy, which is essentially adopted in modern machine learning libraries such as TensorFlow (Abadi et al., 2016) and PyTorch (Paszke et al., 2019), is problematic as it may slow down convergence and result in oscillations. A simple idea to tackle this issue is to bypass the non-smoothness of a regularizer via its proximal operator. This idea is the basis of proximal gradient descent (PGD) methods, which first update the parameter using the gradient of the loss function $f(\theta)$ and then perform a proximal mapping of $\mathcal{R}(\theta)$.

In the *non-stochastic* case, the PGD with both convex and non-convex regularizers has been extensively studied in the literature (Reddi et al., 2016; Allen-Zhu, 2017; Wang et al., 2018; Pham et al., 2019; Chen et al., 2020). Another work, VMFB (Chouzenoux et al., 2014), analyzes the preconditioned gradient descent on convex regularized problems with non-convex loss but does not consider the first-order momentum. In contrast, PGD in the *stochastic* setting has been little explored. Duchi et al. (2011); Ghadimi et al. (2016) consider PGD to solve the stochastic objectives with convex regularizers. Recently, Xu et al. (2019b) studies non-convex and non-smooth regularized problems for DC (difference of convex) functions and Xu et al. (2019a); Davis et al. (2020) present non-asymptotic analysis for non-convex smooth loss and non-convex regularizers, which is the most general setting, but do not consider the preconditioner in the update rule.

All the aforementioned studies of the stochastic case, however, focus either on limited settings (e.g. Duchi et al. (2011) only covers the update rule of ADAGRAD) with convex regularizers only, or on pure vanilla gradient descent for non-convex regularizers. Hence, they cannot accommodate all advanced modern optimization algorithms with *preconditioners*, such as adaptive gradient methods. The only exception is PROX-SGD (Yang et al., 2020), with the caveat that PROX-SGD update rule is *not an exact* PGD. Moreover, the theory in Yang et al. (2020) only guarantees the convergence, *not how fast* Prox-SGD converges, and furthermore this analysis is performed without considering the preconditioners. Table 1 summarizes the previous studies and our work in terms of stochastic PGD. In this paper, we propose an exact framework for stochastic proximal gradient methods with *arbitrary* positive preconditioners and lower semi-continuous (possibly non-convex) regularizers. With our framework, our goal is to provide theoretical and empirical understanding of stochastic proximal gradient methods. Our main contributions are summarized as follows:

 We propose the first general family of stochastic proximal gradient methods, which we term PROXGEN. We introduce two important instances stemming from our approach: (i) the first proximal version of ADAM (Kingma & Ba, 2015) and (ii) a revised version of PROXQUANT (Bai et al., 2019) that improves upon the original approach for quantization-specific regularizers by incorporating the effect of preconditioners when computing proximal mappings.

Algorithm 1 PROXGEN: A General Stochastic Proximal Gradient Method

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1: Input: Stepsize \alpha_t, \{\rho_t\}_{t=1}^{t=T} \in [0,1), regularization parameter \lambda, and small constant 0 < \delta \ll 1.

2: Initialize: \theta_1 \in \mathbb{R}^d, m_0 = 0 \in \mathbb{R}^d, and C_0 = O \in \mathbb{R}^{d \times d}.

3: for t = 1, 2, \ldots, T do

4: Draw a minibatch sample \xi_t from \mathbb{P}

5: g_t \leftarrow \nabla f(\theta_t; \xi_t) \Rightarrow Stochastic gradient at time t \Rightarrow First-order momentum estimate

7: C_t \leftarrow Preconditioner construction

8: \theta_{t+1} \in \underset{\theta \in \Omega}{\operatorname{argmin}} \left\{ \langle m_t, \theta \rangle + \lambda \mathcal{R}(\theta) + \frac{1}{2\alpha_t} (\theta - \theta_t)^\mathsf{T} (C_t + \delta I) (\theta - \theta_t) \right\}

9: end for

10: Output: \theta_{T+1}
```

- We analyze the convergence of the general PROXGEN family and identify essential conditions for convergence. We show that PROXGEN enjoys the same convergence rate as vanilla SGD under mild conditions, and highlight the challenges in our theory and improvements upon previous work. Our convergence guarantee encompasses several existing approaches as special cases.
- In terms of practice, we demonstrate the superiority of proximal methods over subgradient-based
 methods with various non-convex regularizers which have not yet been studied in deep learning.
 Interestingly, our experiments indicate that proximal methods with non-convex regularizers are
 more effective than with convex regularizers for learning sparse deep models.

2 A GENERAL FAMILY OF STOCHASTIC PROXIMAL GRADIENT METHODS

In this section, we present PROXGEN, a general family of stochastic proximal gradient methods, and present both existing and novel instances as showcase examples in our family. Algorithm 1 describes the details of PROXGEN. The update rule on line 8 of Algorithm 1 can be written more compactly:

$$\theta_{t+1} \in \underset{\theta \in \Omega}{\operatorname{argmin}} \left\{ \langle m_t, \theta \rangle + \lambda \mathcal{R}(\theta) + \frac{1}{2\alpha_t} (\theta - \theta_t)^{\mathsf{T}} \Big(C_t + \delta I \Big) (\theta - \theta_t) \right\}$$

$$= \operatorname{prox}_{\alpha_t \lambda \mathcal{R}(\cdot)}^{C_t + \delta I} \Big(\theta_t - \alpha_t (C_t + \delta I)^{-1} m_t \Big)$$
(2)

where the proximal operator in Eq. (2) is defined as $\operatorname{prox}_h^A(z) = \operatorname{argmin}_x\{h(x) + \frac{1}{2}\|x - z\|_A^2\}$. In PROXGEN, we allow both the loss and the regularizer to be non-convex. Now, we introduce possible examples according to the proper combinations of preconditioners C_t and regularizers $\mathcal{R}(\cdot)$.

Existing Instances of PROXGEN. We briefly recover some known examples in PROXGEN family.

- ADAGRAD (Duchi et al., 2011) is the first key instance of adaptive gradient methods where $C_t = (\sum_{\tau=1}^t g_\tau g_\tau^\mathsf{T})^{1/2}$ and $\mathcal{R}(\theta) = \|\theta\|_1$. Any convex regularizer $\mathcal{R}(\cdot)$ is allowed.
- The proximal Newton methods (Lee et al., 2012) employ the exact Hessian $C_t = \nabla^2 f(\theta_t)$ and $\mathcal{R}(\theta) = \|\theta\|_1$. In addition, we can approximate the exact Hessian, which yield proximal Newton-type methods such as quasi-Newton approximation (Becker et al., 2019), L-BFGS approximation (Liu & Nocedal, 1989), and adding a multiple of the identity to the Hessian.

Although the above examples enjoy good theoretical properties in convex settings, many of the modern practical optimization problems involve non-convex loss functions such as learning deep models. Moreover, it is known that non-convex regularizers yield better performance (also in terms of theory) than convex penalties in some applications (see Fu (1998); Park & Yoon (2011); Yang & Lozano (2017); Yun et al. (2019b) and references therein). Considering this motivation and recent advanced optimizers, we arrive at the following new examples.

Novel Instances of PROXGEN. Beyond the well-known methods above, PROXGEN naturally introduces proximal versions of standard SGD techniques developed for solving unregularized problems for deep learning. The following examples are just a few instances that have not been explored so far, and PROXGEN can cover a broader range of new examples depending on the combinations of preconditioners and regularizers.

- The proximal version of ADAM (Kingma & Ba, 2015) with ℓ_q regularization is a possible example where $C_t = \sqrt{\beta C_{t-1} + (1-\beta)g_t^2}$ with $\beta \in [0,1)$ and $\mathcal{R}(\theta) = \|\theta\|_q$ for $0 \le q \le 1$. We mainly validate the superiority of our novel proximal version of ADAM to the usual subgradient-based counterpart empirically in Section 4.
- We can also consider the *proximal* version of KFAC (Martens & Grosse, 2015). For an L-layer neural network, KFAC approximates the Fisher information matrix with layer-wise block diagonal structure where l-th diagonal block $C_{t,[l]}$ corresponds to Kronecker-factored approximation with respect to the parameters at l-th layer. The proximal version of KFAC, which corresponds to $C_{t,[l]} = \mathbb{E}[\delta_l \delta_l^\mathsf{T}] \otimes \mathbb{E}[a_{l-1} a_{l-1}^\mathsf{T}]$ and $\mathcal{R}(\theta) = \|\theta\|_q$ where δ_l is the gradient with respect to the outputs of l-th layer and a_{l-1} is the activation of (l-1)-th layer, could be another example.

Examples of Proximal Mappings for PROXGEN. We provide update rules for PROXGEN with ℓ_q regularization $(0 \le q \le 1)$ and diagonal preconditioners. Diagonal preconditioners are used by popular adaptive gradient methods such as ADAM. Specifically, we consider regularizer $\mathcal{R}(\theta) = \lambda \sum_{j=1}^p |\theta_j|^q$ for $\theta \in \mathbb{R}^p$ with diagonal preconditioner matrix C_t . Note that for $C_t = I$ (i.e. vanilla gradient descent), it is known that closed-form solutions exist for proximal mappings for $q \in \{0, \frac{1}{2}, \frac{2}{3}, 1\}$ (Cao et al., 2013). We denote the *i*-th coordinate of the vector θ_t as $\theta_{t,i}$ and the diagonal entry $[C_t]_{ii}$ as $C_{t,i}$

• ℓ_1 regularization. The proximal mappings for the case of ℓ_1 regularization with preconditioner can be computed efficiently via soft-thresholding as

$$\widehat{\theta}_{t,i} = \theta_{t,i} - \alpha_t \frac{m_{t,i}}{C_{t,i} + \delta}, \quad \theta_{t+1,i} = \operatorname{sign}(\widehat{\theta}_{t,i}) \left(\left| \widehat{\theta}_{t,i} \right| - \frac{\alpha_t \lambda}{C_{t,i} + \delta} \right)$$
(3)

• ℓ_0 regularization. In case of ℓ_0 regularization, we can compute the closed-form solutions via hard-thresholding as

ding as
$$\widehat{\theta}_{t,i} = \theta_{t,i} - \alpha_t \frac{m_{t,i}}{C_{t,i} + \delta}, \quad \theta_{t+1,i} = \begin{cases}
\widehat{\theta}_{t,i}, & |\widehat{\theta}_{t,i}| > \sqrt{\frac{2\alpha_t \lambda}{C_{t,i} + \delta}}, \\
0, & |\widehat{\theta}_{t,i}| < \sqrt{\frac{2\alpha_t \lambda}{C_{t,i} + \delta}}, \\
\{0, \widehat{\theta}_{t,i}\}, & |\widehat{\theta}_{t,i}| = \sqrt{\frac{2\alpha_t \lambda}{C_{t,i} + \delta}}
\end{cases} \tag{4}$$

The closed-form proximal mappings for $\ell_{1/2}$ and $\ell_{2/3}$ regularization are provided in the Appendix.

Revised PROXQUANT (Bai et al., 2019). The recently proposed PROXQUANT proposes novel regularizations for network quantization. Especially for binary quantization, a W-shaped regularizer is defined as $\mathcal{R}_{\rm bin}(\theta) = \|\theta - {\rm sign}(\theta)\|_1$ where ${\rm sign}(\theta)$ is applied on

Table 2: PROXQUANT versus revised PROXQUANT
$$\frac{\text{PROXQUANT} \left\| \text{prox}_{\alpha_t \lambda \mathcal{R}(\cdot)} \left(\theta_t - \alpha_t (C_t + \delta I)^{-1} m_t \right) \right\|}{\text{Revised}} \frac{\text{Revised}}{\text{PROXQUANT}} \left\| \text{prox}_{\alpha_t \lambda \mathcal{R}(\cdot)}^{C_t + \delta I} \left(\theta_t - \alpha_t (C_t + \delta I)^{-1} m_t \right) \right\|}$$

 θ in an element-wise manner. Using this regularizer, the main difference between PROXQUANT and our PROXGEN approach is shown in Table 2. Note that PROXQUANT (top in Table 2) does not consider the effect of preconditioners when computing proximal mappings. Therefore, we revise the proximal update in PROXQUANT by considering preconditioners in proximal mappings with PROXGEN (bottom in Table 2). Moreover, we also propose *generalized regularizers* motivated by ℓ_q regularization for 0 < q < 1: $\mathcal{R}_{\text{bin}}^q(\theta) = \|\theta - \text{sign}(\theta)\|_q$. In terms of theory, Bai et al. (2019) prove the convergence of PROXQUANT only for the *full-batch* gradient with *differentiable* regularizers, which is also guaranteed only for vanilla gradient descent. In contrast, using our *revised* PROXQUANT, we can completely bridge the gap in theory (via Theorem 1 in Section 3, which is stated for *stochastic* optimization), and we provide the *exact* update rule for solving problem in Eq. (1). We also investigate the empirical differences of PROXQUANT and our revised PROXQUANT in Section 4.

3 Convergence Analysis

In this section, we provide convergence guarantees for the PROXGEN family. Our goal is to find an ϵ -stationary point for the problem in Eq. (1) where ϵ is the required precision. For notational convenience, we assume that the regularization parameter λ is incorporated into $\mathcal{R}(\theta)$ in Eq. (1). To guarantee the convergence under this setting, we should deal with the subdifferential defined as:

Definition 1 (Fréchet Subdifferential). Let φ be a real-valued function. The Fréchet subdifferential $\text{of } \varphi \text{ at } \bar{\theta} \text{ with } |\varphi(\bar{\theta})| < \infty \text{ is defined by } \widehat{\partial} \varphi(\bar{\theta}) \coloneqq \{\theta^* \in \Omega \ \Big| \ \liminf_{\theta \to \bar{\theta}} \frac{\varphi(\theta) - \varphi(\bar{\theta}) - \langle \theta^*, \theta - \bar{\theta} \rangle}{\|\theta - \bar{\theta}\|} \ge 0\}.$

To derive the convergence bound, we make the following mild conditions:

- (C-1) (L-smoothness) The loss function f is differentiable, L-smooth, and lower-bounded: $\forall x, y, \|\nabla f(x) - \nabla f(y)\| \le L\|x - y\|$ and $f(x^*) > -\infty$ for the optimal solution x^* .
- (C-2) (Bounded variance) The stochastic gradient $g_t = \nabla f(\theta_t; \xi)$ is unbiased and has the bounded variance: $\mathbb{E}_{\xi} [\nabla f(\theta_t; \xi)] = \nabla f(\theta_t), \quad \mathbb{E}_{\xi} [\|g_t - \nabla f(\theta_t)\|^2] \leq \sigma^2.$
- (C-3) (i) final step-vector is finite, (ii) the stochastic gradient is bounded, and (iii) the momentum parameter should be exponentially decaying: (i) $\|\theta_{t+1} - \theta_t\| \le D$, (ii) $\|g_t\| \le G$, (iii) $\rho_t =$ $\rho_0 \mu^{t-1}$ with D, G > 0 and $\rho_0, \mu \in [0, 1)$.
- (C-4) (Sufficiently positive-definite) The minimum eigenvalue of effective spectrums should be uniformly lower bounded over all time $t: \forall t, \ \lambda_{\min}(\alpha_t(C_t + \delta I)^{-1}) \geq \gamma > 0.$

(C-1) and (C-2) are standard in general non-convex optimization (Ghadimi & Lan, 2013; Ghadimi et al., 2016; Zaheer et al., 2018; Xu et al., 2019a). In addition, (C-3) is extensively studied in previous literature in the context of adaptive gradient methods (Kingma & Ba, 2015; Reddi et al., 2018; Chen et al., 2019a). Lastly, a similar condition to (C-4) is also considered in Chen et al. (2019a); Yun et al. (2019a), and it can be easily satisfied in practice. More discussion on (C-4) is provided later.

Since the loss function f is assumed to be differentiable as in (C-1), we have, at stationary points, $\mathbf{0} \in \partial F(\theta) = \nabla f(\theta) + \partial \mathcal{R}(\theta)$, so the convergence criterion is slightly different from that of general non-convex optimization. Hence, we use the following convergence criterion $\mathbb{E}[\operatorname{dist}(\mathbf{0}, \partial F(\theta))] \leq \epsilon$ for an ϵ -stationary point where $\operatorname{dist}(x,A)$ denotes the distance between a vector x and a set A. If no regularizer is considered ($\mathcal{R}=0$), this criterion boils down to the one usually used in non-convex optimization, $\mathbb{E}[\|\nabla f(\theta)\|] \leq \epsilon$. We are now ready to state our main theorem for general convergence.

Theorem 1. Let θ_a denote an iterate uniformly randomly chosen from $\{\theta_1, \dots, \theta_T\}$. Under the conditions (C-1), (C-2), (C-3), (C-4) with the initial stepsize $\alpha_0 \leq \frac{\delta}{3L}$ and non-increasing stepsize α_t , PROXGEN, Algorithm I, is guaranteed to yield $\mathbb{E}_a[\operatorname{dist}(\mathbf{0},\widehat{\partial}F(\theta_a))^2] \leq \frac{Q_1\sigma^2}{T}\sum_{t=0}^{T-1}\frac{1}{b_t}+\frac{Q_2\Delta}{T}+\frac{Q_3}{T}$ where $\Delta=f(\theta)-f(\theta^*)$ with optimal point θ^* , and b_t is the minibatch size at time t. The constants $\{Q_i\}_{i=1}^3$ on the right-hand side depend on the constants $\{\alpha_0, \delta, L, D, G, \rho_0, \mu, \gamma\}$, but not on T.

From Theorem 1, the appropriate minibatch size is important to ensure a good convergence. Various settings for the minibatch size could be employed for convergence guarantee (for example, $b_t = t$), but considering practical cases, we provide the following important corollary for *constant minibatch*.

Corollary 1 (Constant Mini-batch). Under the same assumptions as in Theorem 1 with sample size n and constant minibatch size $b_t = b = \Theta(T) = \Theta(\sqrt{n})$, we have $\mathbb{E}\left[\operatorname{dist}(\mathbf{0},\widehat{\partial}F(\theta_a))^2\right] \leq \mathcal{O}(1/T)$ and the total complexity is $\mathcal{O}(1/\epsilon^4)$ in order to have $\mathbb{E}[\operatorname{dist}(\mathbf{0},\widehat{\partial}F(\theta_a))] \leq \epsilon$.

Here we make several remarks on our results and relationship with prior work.

• Improvements upon Prior Work. The most challenging parts in our analysis compared to previous study (Xu et al., 2019a) (which is only for vanilla SGD) is that we should handle the momentum m_t and non-trivial preconditioner C_t . Due to the existence of m_t , it is highly non-trivial to bound the term $||m_t - \nabla f(\theta_t)||_2$ without suitable assumptions whereas $||g_t - \nabla f(\theta_t)||_2$ in Xu et al. (2019a) can be easily bounded using (C-2). The second challenge is to deal with quadratic approximation term $(\theta - \theta_t)^{\mathsf{T}} (C_t + \delta I)(\theta - \theta_t)$ in Algorithm 1 which is not problematic in Xu et al. (2019a) due to trivial $C_t = I$. We can successfully bypass those difficulties using mild conditions (C-3) and (C-4) respectively and also allow *non-increasing* stepsize.

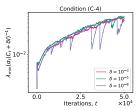


Figure 1: Empirical results for condition (C-4).

• On Condition (C-4). (C-4) is easily satisfied both theoretically and empirically. Most of the popular optimization algorithms for deep learning such as ADAGRAD, ADAM, and KFAC satisfies this condition (see Appendix D). In order to investigate whether this condition could be satisfied in real problems, we train ResNet-34 on CIFAR-10 dataset. In Figure 1, we can see the minimum eigenvalue of $\alpha_t(C_t + \delta I)^{-1}$ tends to increase, so the condition (C-4) is also satisfied empirically.

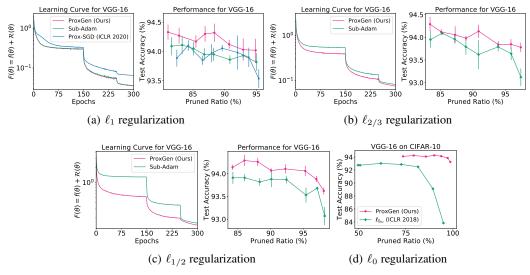


Figure 2: Comparison for sparse VGG-16 on CIFAR-10 dataset.

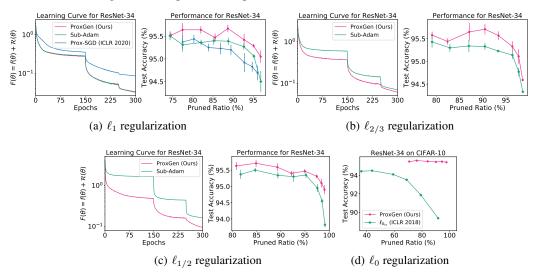


Figure 3: Comparison for sparse ResNet-34 on CIFAR-10 dataset.

- Implications of Condition (C-4) on Theory. Our analysis relies on (C-4), the lower bound for the minimum eigenvalue of $\Gamma_t := \alpha_t (C_t + \delta I)^{-1}$. This means that Theorem 1 guarantees $\mathbb{E}_a[\mathrm{dist}(\mathbf{0},\widehat{\partial}F(\theta_a)^2] \leq \mathcal{O}(1/\sqrt{T})$ (in case of $b = \Theta(\sqrt{n})$ as in Corollary 1) for *any* change of basis of Γ_t , so in that sense, we provide a worst-case analysis and there is room for more optimistic bounds.
- Connections to Second-order Methods. Our analysis can provide guarantees for *positive* second-order preconditioners as long as (C-4) is satisfied (The empirical Fisher information (Martens & Grosse, 2015) is one example). Although second-order solvers generally enjoy very fast convergence under strongly convex loss (Lee et al., 2012; Zhang et al., 2019), it can be understood that our theory guarantees at least a sublinear rate for such second-order curvatures with less stringent conditions.

4 EXPERIMENTS

We consider two important tasks for regularized training in deep learning communities: (i) training sparse neural networks and (ii) network quantization. Throughout our experiments, we consider ADAM as a representative of PROXGEN where $m_t = \rho_t m_{t-1} + (1-\rho_t)g_t$ with constant decaying parameter $\rho_t = 0.9$ and $C_t = \sqrt{\beta C_{t-1} + (1-\beta)g_t^2}$ with $\beta = 0.999$ in Algorithm 1. The details on other hyperparameter/experiment settings are provided in the Appendix.

Table 3: Comparison for binary neural networks. The best performance in mean value is highlighted.

Test Error (%)

1600 20101 (70)								
Baselines			PROXGEN (Ours)					
Model	Full Precision (32-bit)	BinaryConnect Courbariaux et al. (2015)	PROXQUANT Bai et al. (2019)			Revised ProxQuant $\ell_{1/2}$		
ResNet-20	8.06	9.54 ± 0.03	9.35 ± 0.13	9.50 ± 0.12	9.72 ± 0.06	9.78 ± 0.18		
ResNet-32	7.25	8.61 ± 0.27	8.53 ± 0.15	8.29 ± 0.07	8.22 ± 0.05	8.43 ± 0.15		
ResNet-44	6.96	8.23 ± 0.23	7.95 ± 0.05	7.68 ± 0.07	7.91 ± 0.08	7.90 ± 0.13		
ResNet-56	6.54	7.97 ± 0.22	7.70 ± 0.06	7.52 ± 0.18	7.60 ± 0.09	7.61 ± 0.12		

Training Sparse Neural Networks. Motivated by the lottery ticket hypothesis (Frankle & Carbin, 2019), we consider training VGG-16 (Simonyan & Zisserman, 2014) and ResNet-34 (He et al., 2016) on CIFAR-10 dataset using sparsity encouraging regularizers. Toward this, we consider the following objective function with ℓ_q regularization: $F(\theta) \coloneqq \mathbb{E}_{\xi \sim \mathbb{P}}[f(\theta; \xi)] + \lambda \sum_{j=1}^p |\theta_j|^q$ where $0 \le q \le 1$. We train the network parameters with the closed-form proximal mappings introduced in Section 2.

We compare PROXGEN with subgradient methods and also include PROX-SGD (Yang et al., 2020) as a baseline especially for ℓ_1 regularization since PROX-SGD considers only convex regularizers. In PROX-SGD, the hand-crafted fine-tuned scheduling on α_t and ρ_t is essential for fast convergence and good performance, but in our experiments we use standard settings $\rho_t = 0.9$ with step-decay learning rate scheduling for fair comparisons. For ℓ_0 regularization, the problem in Eq. (1) cannot be optimized in a subgradient manner, so we compare PROXGEN with another popular baseline, ℓ_{0hc} (Louizos et al., 2018) which approximates the ℓ_0 -norm via hard-concrete distributions.

Figures 2 and 3 illustrate the results for VGG-16 and ResNet-34 respectively. In terms of convergence, PROXGEN shows faster convergence than PROX-SGD for ℓ_1 case, but there is no difference between PROXGEN and subgradient methods. However, there are notable differences in convergence for non-convex regularizers $\ell_{1/2}$ and $\ell_{2/3}$, which get bigger as q decreases. We believe this might be because the ℓ_q -norm derivative, $q/|\theta|^{1-q}$, is very large for non-zero tiny θ for $q \in (0,1)$. Meanwhile, $\partial |\theta|/\partial \theta$ is merely the sign value regardless of size of θ , so the large gradient of $|\theta|^q$ may hinder convergence. The learning curves in Figure 2-(b,c) and 3-(b,c) empirically corroborate this phenomenon.

In terms of performance, we can see that PROXGEN consistently achieves better performance than baselines for both VGG-16 and ResNet-34 with similar or even better sparsity level. Importantly, PROXGEN with ℓ_0 outperforms $\ell_{0_{hc}}$ baseline by a great margin. This might be due to the design of $\ell_{0_{hc}}$, which approximates $\|\theta\|_0 = \sum_{j=1}^p \mathbb{I}\{\theta_j \neq 0\}$ with binary mask z_j parameterized by learnable probability π_j for each coordinate. Thus, the number of parameters to be optimized is doubled, which might make optimization harder. In constrast, PROXGEN does not introduce additional parameters.

More results for MCP (Zhang et al., 2010) and SCAD (Fan & Li, 2001) regularizers are in Appendix.

Training Binary Neural Networks. In the second set of experiments, we consider the network quantization constraining the parameters to some set of discrete values which is a key approach for model compression. We evaluate our revised PROXQUANT in Table 2 with extended regularization $\mathcal{R}^q_{\rm bin}$ in Section 2. We consider the following objective function with quantization-specific regularizers: $F(\theta) \coloneqq \mathbb{E}_{\xi \sim \mathbb{P}}[f(\theta; \xi)] + \lambda \sum_{j=1}^p |\theta_j - \mathrm{sign}(\theta_j)|^q$ where $0 \le q \le 1$. For comparisons, we quantize ResNet on CIFAR-10 dataset and follow the same experiment settings as in PROXQUANT.

Table 3 presents the results. For all q values, revised PROXQUANT consistently outperforms the baselines except for ResNet-20, which implies PROXGEN may work better for larger networks. As such, our generalized regularizers $\mathcal{R}^q_{\mathrm{bin}}$ contribute to one of the state-of-the-art optimization-based methods in network quantization. Notably, revised PROXQUANT ℓ_1 greatly outperforms PROXQUANT baseline while these two approaches differ only in update rules (see Table 2). Hence, we can conclude that revised PROXQUANT based on PROXGEN provides an *exact* proximal update and also yields more generalizable solutions. In our experience, revised PROXQUANT ℓ_0 shows little degradation in performance, so we do not include this result. However, revised PROXQUANT ℓ_0 shows superiority to baselines for language modeling, whose preliminary results are in Appendix.

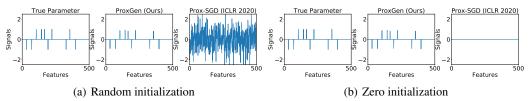


Figure 4: Lasso simulations with different initialization schemes.

5 A CLOSER LOOK INTO PROX-SGD (YANG ET AL., 2020) VS. PROXGEN

Prox-SGD (Yang et al., 2020) is the approach closest to our PROXGEN method. However, PROX-SGD is *not an exact* proximal approach and is significantly different from PROXGEN. PROXGEN's update rule involves directly solving the quadratic subproblem (Eq. (2)). In contrast, PROX-SGD's update rule consists of two stages: (i) solving the quadratic subproblem *without* learning rate, then (ii) updating the parameters with the computed direction (i.e. $\hat{\theta}_t - \theta_t$) by the learning rate α_t (Eq. (5)).

$$\widehat{\theta}_t = \underset{\theta \in \Omega}{\operatorname{argmin}} \left\{ \langle m_t, \theta \rangle + \lambda \mathcal{R}(\theta) + \frac{1}{2} (\theta - \theta_t)^{\mathsf{T}} \Big(C_t + \delta I \Big) (\theta - \theta_t) \right\}, \ \theta_{t+1} = \theta_t + \alpha_t (\widehat{\theta}_t - \theta_t)$$
 (5)

To clearly see the differences between both approaches, we conduct two studies.

Study 1: Lasso Support Recovery. For this task, the two-stage update scheme of PROX-SGD might have some potential issues. For example, for ℓ_1 -regularized problems, the updated parameter θ_{t+1} (Eq. (5)) might not achieve exact zero (while $\widehat{\theta}_t$ can) whereas θ_{t+1} for PROXGEN (Eq. (2)) can attain exact zero value according to the update rule (Eq. (3)) in Section 2. Another potential caveat is that PROX-SGD might overestimate the sparsity level. In view of the above, we run Lasso simulations with different two initialization schemes: (i) random initialization and (ii) zero initialization. For random initialization, it can be seen in Figure 4-(a) that PROX-SGD could not achieve exact zero value, which corroborates our first observation. More interestingly, for zero initialization, we can see in Figure 4-(b) that the estimates using PROX-SGD are exactly zeros for all coordinates, which supports our second observation. This might be because $\widehat{\theta}_t$ (Eq. (5)) is always zero since the quadratic subproblem does not consider the learning rate, which might overestimate the sparsity level. Hence, the subsequent iterate θ_{t+1} would be always zero since we initialize the parameters with zeros. On the other hand, PROXGEN correctly recovers the support in both cases.

Study 2: DenseNet-201 on CIFAR-100 Dataset. To validate the superiority of PROXGEN upon PROX-SGD, we revisit the largest experiments in Yang et al. (2020). We train DenseNet-201 architecture on CIFAR-100 dataset with ℓ_1 regularization since PROX-SGD only consider convex regularizers. For both methods, we use the same hyperparameter settings for fair comparison. Figure 5 illustrates the training learning curves, and it can be seen that our PROXGEN achieves faster convergence as well as lower objective values. For our experience, the learning curves show the similar dynamics for different λ values.

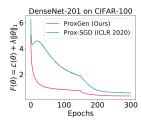


Figure 5: Learning curve.

Comparison of Theoretical Contributions. Yang et al. (2020) guarantees the convergence of PROX-SGD, but *not how fast* it converges. Moreover, this is proved *without* considering preconditioners. In contrast, our analysis for the PROXGEN framework appropriately incorporates the first-order momentum and arbitrary positive preconditioner with detailed non-asymptotic convergence.

6 CONCLUSION

In this work, we proposed PROXGEN, the first general family of stochastic proximal gradient methods. Within our framework, we presented novel examples of proximal versions of standard SGD approaches, including a proximal version of ADAM. We analyzed the convergence of the whole PROXGEN family and showed that PROXGEN can encompass the results of several previous studies. We also demonstrated that PROXGEN empirically outperforms subgradient-based methods for popular deep learning problems. As future work, we plan to study efficient approximations of proximal mappings for structured regularizers such as ℓ_1/ℓ_q norms with preconditioners.

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APPENDIX

A ADDITIONAL EXPERIMENTS: SPARSE NEURAL NETWORKS WITH MCP AND SCAD NON-CONVEX REGULARIZERS

We provide the additional experiments for sparse neural networks with MCP (Zhang et al., 2010) and SCAD (Fan & Li, 2001) non-convex regularizers. Figure 6 and 7 illustrate the results for VGG-16 and ResNet-34 respectively. As shown in Section 4 and these figures, PROXGEN is very effective for solving the non-convex regularized problems.

B DETAILS ON EXPERIMENTAL SETTINGS

Sparse Neural Networks. To reflect the most practical training settings, we first tune the weight-decay parameter ζ without ℓ_q regularizers. For weight-decay coefficients, we consider the candidates $\zeta \in \{0.001, 0.002, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2, 0.5\}$ for ζ and the best ζ value is 0.2 for both networks VGG-16 and ResNet-34 in our experience. After tuning weight-decay coefficient ζ , we consider both decoupled weight decay (Loshchilov & Hutter, 2019) and ℓ_q regularization whose detail update rule is described in Algorithm 2. For all comparison methods except $\ell_{0_{hc}}$, the recommended stepsize $\alpha_t = 0.001$ is employed, but we tune this stepsize for $\ell_{0_{hc}}$ baseline. We consider a broad range of regularization parameters for all methods: $\lambda \in \{0.001, 0.002, 0.005, 0.01, 0.02, \cdots, 1.0, 2.0, 5.0\}$. With these hyperparameter settings, we consider the total 300 epochs and divide the learning rate at 150-th and 250-th epoch by 10.

Binary Neural Networks. In this experiment, we follow the same experimental settings in baseline PROXQUANT (Bai et al., 2019). We first pre-train ResNet- $\{20, 32, 44, 56\}$ with full-precision and initialize the network parameters with these pre-trained weights. Then, we consider the total 300 epochs and hard-quantize the networks at 200-th epoch (i.e. quantizing the weight parameters to +1 or -1). We employ the homotopy method introduced in Bai et al. (2019): annealing the regularization parameter λ as $\lambda_{\rm epoch} = \lambda \times {\rm epoch}$. For initial value of λ , we use $\lambda = 10^{-8}$ or $\lambda = 5 \cdot 10^{-8}$ for all ResNet architecture. We use the constant stepsize $\alpha_t = 0.01$ as recommended in Bai et al. (2019).

Lasso Support Recovery. We generate simple Lasso simulations with problem dimension p=500 and n=100 data samples. The number of non-zero entries in true parameter vector $\theta^* \in \mathbb{R}^p$ is set to 10. The design matrix $X \in \mathbb{R}^{n \times p}$ is generated from standard Gaussian distribution $\mathcal{N}(0,1)$ and we randomly assign +1 or -1 for the non-zero value in true parameter at random 10 coordinates. The response variable $y \in \mathbb{R}^n$ is generated with small noise by $y = X\theta^* + \epsilon$ where $\epsilon \sim \mathcal{N}(0,0.05^2)$. For both PROXGEN and PROX-SGD, we employ ADAM for preconditioner matrix C_t construction.

Here, we introduce preliminary results of revised PROXQUANT ℓ_0 on language modeling. For this experiment, we train one hidden layer LSTM with embedding dimension 300 and 300 hidden units according to Bai et al. (2019). First, we pre-train the full-precision LSTM and initialize the network with pre-trained weights. We consider the total 80 epochs and divide the learning rate by 1.2 if the validation loss does not decrease. Table 4 shows the preliminary results and revised PROXQUANT ℓ_0 is superior to the PROXQUANT baseline in this task.

Table 4: Preliminary results on revised PROXQUANT ℓ_0 for LSTM models.

Algorithm	Test Perplexity	
Full-precision (32-bit)	88.5	
BinaryConnect Courbariaux et al. (2015) PROXQUANT Bai et al. (2019)	372.2 288.5	
revised ProxQuant ℓ_0 (Ours)	223.4	

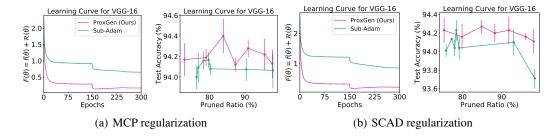


Figure 6: Comparison for sparse VGG-16 on CIFAR-10 dataset with other non-convex regularizers.

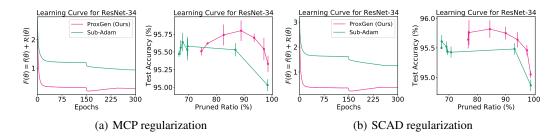


Figure 7: Comparison for sparse ResNet-34 on CIFAR-10 dataset with other non-convex regularizers.

C DERIVATIONS FOR PROXIMAL MAPPINGS

Here, we derive the concrete update rule for ℓ_q regularization with *diagonal* preconditioners as introduced in Section 2.

 $\ell_{1/2}$ **regularization.** First, we review the closed-form proximal mappings for $\ell_{1/2}$ regularization of vanilla SGD. First, we consider the following one-dimensional program:

$$\widehat{x} = \underset{\longrightarrow}{\operatorname{argmin}} \{ (x - z)^2 + \lambda |x|^{1/2} \}$$
(6)

For the program Eq. (6), it is known that the closed-form solution exists Cao et al. (2013) as

$$\widehat{x} = \begin{cases} \frac{2}{3} |z| \left(1 + \cos\left(\frac{2}{3}\pi - \frac{2}{3}\varphi_{\lambda}(z)\right) \right) & \text{if } z > p(\lambda) \\ 0 & \text{if } |z| \le p(\lambda) \\ -\frac{2}{3} |z| \left(1 + \cos\left(\frac{2}{3}\pi - \frac{2}{3}\varphi_{\lambda}(z)\right) \right) & \text{if } z < -p(\lambda) \end{cases}$$

$$(7)$$

where $\varphi_{\lambda}(z) = \arccos\left(\frac{\lambda}{8}\left(\frac{|z|}{3}\right)^{-3/2}\right)$ and $p(\lambda) = \frac{\sqrt[3]{54}}{4}(\lambda)^{2/3}$. Based on this closed-form solution, we derive PROXGEN for $\ell_{1/2}$ regularization with diagonal preconditioners. By Eq. (2), we have

$$\widehat{\theta}_t = \theta_t - \alpha_t (C_t + \delta I)^{-1} m_t \tag{8}$$

$$\theta_{t+1} \in \operatorname{prox}_{\alpha_t \lambda \mathcal{R}(\cdot)}^{C_t + \delta I}(\widehat{\theta}_t)$$
 (9)

$$= \underset{\theta}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\theta - \widehat{\theta}_t\|_{C_t + \delta I}^2 + \lambda \sum_{j=1}^p |\theta_j|^{1/2} \right\}$$
 (10)

Since the program Eq. (10) is coordinate-wise decomposable (since the preconditioner matrix C_t is diagonal), we can split Eq. (10) into

$$\theta_{t+1,i} = \underset{\theta_i}{\operatorname{argmin}} \left\{ \frac{1}{2} (C_{t,i} + \delta) (\theta_i - \widehat{\theta}_{t,i})^2 + \alpha_t \lambda |\theta_i|^{1/2} \right\}$$
$$= \underset{\theta_i}{\operatorname{argmin}} \left\{ (\theta_i - \widehat{\theta}_{t,i})^2 + \frac{2\alpha_t \lambda}{C_{t,i} + \delta} |\theta_i|^{1/2} \right\}$$

for the i-th coordinate. From Eq. (6), we can derive

$$\theta_{t+1,i} = \begin{cases} \frac{2}{3} |\widehat{\theta}_{t,i}| \left(1 + \cos\left(\frac{2}{3}\pi - \frac{2}{3}\varphi_{\lambda}(\widehat{\theta}_{t,i})\right) \right) & \text{if } \widehat{\theta}_{t,i} > p(\lambda) \\ 0 & \text{if } |\widehat{\theta}_{t,i}| \le p(\lambda) \\ -\frac{2}{3} |\widehat{\theta}_{t,i}| \left(1 + \cos\left(\frac{2}{3}\pi - \frac{2}{3}\varphi_{\lambda}(\widehat{\theta}_{t,i})\right) \right) & \text{if } \widehat{\theta}_{t,i} < -p(\lambda) \end{cases}$$

where

$$\varphi_{\lambda}(\widehat{\theta}_{t,i}) = \arccos\left(\frac{\alpha_t \lambda}{4(C_{t,i} + \delta)} \left(\frac{|\widehat{\theta}_{t,i}|}{3}\right)^{-3/2}\right), \quad p(\lambda) = \frac{\sqrt[3]{54}}{4} \left(\frac{2\alpha_t \lambda}{C_{t,i} + \delta}\right)^{2/3}.$$

 $\ell_{2/3}$ **regularization.** Now, we provide the closed-form solutions for proximal $\ell_{2/3}$ mappings with diagonal preconditioners. Similar to $\ell_{1/2}$ regularization, we start from the closed-form solutions of the following program:

$$\widehat{x} = \underset{\tau}{\operatorname{argmin}} \{ (x - z)^2 + \lambda |x|^{2/3} \}$$
(11)

The closed-form solution for the program Eq. (11) is known to be

$$\widehat{x} = \begin{cases} \left(\frac{|A| + \sqrt{\frac{2|z|}{|A|} - |A|^2}}{2}\right)^3 & \text{if } z > \frac{2}{3}\sqrt[4]{3\lambda^3} \\ 0 & \text{if } |z| \le \frac{2}{3}\sqrt[4]{3\lambda^3} \\ -\left(\frac{|A| + \sqrt{\frac{2|z|}{|A|} - |A|^2}}{2}\right)^3 & \text{if } z < -\frac{2}{3}\sqrt[4]{3\lambda^3} \end{cases}$$
(12)

where

$$|A| = \frac{2}{\sqrt{3}} \lambda^{1/4} \left(\cosh\left(\frac{\phi}{3}\right) \right)^{1/2}, \quad \phi = \operatorname{arccosh}\left(\frac{27z^2}{16}\lambda^{-3/2}\right)$$
 (13)

Based on this formulation, we derive the closed-form proximal mappings with diagonal preconditioner C_t . By Eq. (2), we have

$$\widehat{\theta}_t = \theta_t - \alpha_t (C_t + \delta I)^{-1} m_t \tag{14}$$

$$\theta_{t+1} \in \operatorname{prox}_{\alpha_t \lambda \mathcal{R}(\cdot)}^{C_t + \delta I}(\widehat{\theta}_t)$$
 (15)

$$= \underset{\theta}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\theta - \widehat{\theta}_t\|_{C_t + \delta I}^2 + \lambda \sum_{j=1}^p |\theta_j|^{2/3} \right\}$$
 (16)

As in $\ell_{1/2}$ case, the program Eq. (16) is coordinate-wise separable, so it suffices to solve the sub-problems for each coordinate as

$$\theta_{t+1,i} = \underset{\theta_i}{\operatorname{argmin}} \left\{ \frac{1}{2} (C_{t,i} + \delta)(\theta_i - \widehat{\theta}_i)^2 + \alpha_t \lambda |\theta_i|^{2/3} \right\}$$
$$= \underset{\theta_i}{\operatorname{argmin}} \left\{ (\theta_i - \widehat{\theta}_{t,i})^2 + \frac{2\alpha_t \lambda}{C_{t,i} + \delta} |\theta_i|^{2/3} \right\}$$

From Eq. (11), we can derive

$$\theta_{t+1,i} = \begin{cases} \left(\frac{|A| + \sqrt{\frac{2|\widehat{\theta}_{t,i}|}{|A|}} - |A|^2}{2}\right)^3 & \text{if } \widehat{\theta}_{t,i} > \frac{2}{3}\sqrt[4]{3\lambda^3} \\ 0 & \text{if } |\widehat{\theta}_{t,i}| \le \frac{2}{3}\sqrt[4]{3\lambda^3} \\ -\left(\frac{|A| + \sqrt{\frac{2|\widehat{\theta}_{t,i}|}{|A|}} - |A|^2}{2}\right)^3 & \text{if } \widehat{\theta}_{t,i} < -\frac{2}{3}\sqrt[4]{3\lambda^3} \end{cases}$$

where

$$|A| = \frac{2}{\sqrt{3}} \left(\frac{2\alpha_t \lambda}{C_{t,i} + \delta}\right)^{1/4} \left(\cosh\left(\frac{\phi}{3}\right)\right)^{1/2}, \quad \phi = \operatorname{arccosh}\left(\frac{27\widehat{\theta}_{t,i}^2}{16} \left(\frac{2\alpha_t \lambda}{C_{t,i} + \delta}\right)^{-3/2}\right)$$

In addition to ℓ_q regularization, we provide the closed-form proximal mappings for another regularizers with non-trivial preconditioners.

MCP regularization. Before introducing the closed-form of proximal m mappings for MCP regularized problems with diagonal preconditioners, we first review the MCP regularizer. The MCP regularizer is defined as

$$\rho_{\lambda}(x;b) = \begin{cases} \lambda |x| - \frac{x^2}{2b} & \text{if } |x| \le b\lambda\\ \frac{b\lambda^2}{2} & \text{if } |x| > b\lambda \end{cases}$$
(17)

where b > 0 is called the MCP parameter and λ is a regularization parameter. Our goal is to derive the proximal mapping of this regularizer with diagonal preconditioner.

Now, we start from the closed-form solutions of the following program:

$$\widehat{x} = \underset{x}{\operatorname{argmin}} \left\{ \frac{1}{2} (x - z)^2 + \rho_{\lambda}(x; b) \right\}$$
(18)

For this program, the closed-form solution is known as

$$\widehat{x} = \operatorname{sign}(z) \min\left\{ \frac{b \max\{|z| - \lambda, 0\}}{b - 1}, |z| \right\}$$
(19)

Based on this closed-form solution, we derive the closed-form proximal mappings with diagonal preconditioner C_t . By Eq. (2), we have

$$\widehat{\theta}_t = \theta_t - \alpha_t (C_t + \delta I)^{-1} m_t \tag{20}$$

$$\theta_{t+1} \in \operatorname{prox}_{\alpha_t \rho_{\lambda}(\cdot; b)}^{C_t + \delta I}(\widehat{\theta}_t)$$
 (21)

$$= \underset{\theta}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\theta - \widehat{\theta}_t\|_{C_t + \delta I}^2 + \alpha_t \rho_{\lambda}(\theta; b) \right\}$$
 (22)

Since this program is also coordinate-wise separable, we could have for each coordinate

$$\theta_{t+1,i} = \operatorname{sign}(\widehat{\theta}_{t,i}) \min \left\{ \frac{b \max\{|\widehat{\theta}_{t,i}| - \frac{\alpha_t \lambda}{C_{t,i} + \delta}, 0\}}{b - 1}, |\widehat{\theta}_{t,i}| \right\}$$
(23)

SCAD regularization. We first introduce SCAD regularizer defined as:

$$\rho_{\lambda}(x;a) = \begin{cases} \lambda|x| & \text{if } |x| \le \lambda \\ \frac{-\lambda^2 - 2a\lambda|x| + x^2}{2(a-1)} & \text{if } \lambda < |x| \le a\lambda \\ \frac{(a+1)\lambda^2}{2} & \text{if } |x| > a\lambda \end{cases}$$
(24)

where a>2 is called the SCAD parameter and λ is a regularization parameter. As in MCP regularizer, we start from the following program

$$\widehat{x} = \underset{x}{\operatorname{argmin}} \left\{ \frac{1}{2} \|x - z\|^2 + \rho_{\lambda}(x; a) \right\}$$

The closed-form solution for this program is known as

$$\widehat{x} = \begin{cases} \operatorname{sign}(z) \max\{|z| - \lambda, 0\} & \text{if } |z| \le 2\lambda \\ \frac{(a-1)z - \operatorname{sign}(z)a\lambda}{a-2} & \text{if } 2\lambda < |z| \le a\lambda \\ z & \text{if } |z| > a\lambda \end{cases}$$
 (25)

Based on this formulation, we could derive the closed-form solution for PROXGEN with diagonal preconditioner. By Eq. (2), we have

$$\widehat{\theta}_t = \theta_t - \alpha_t (C_t + \delta I)^{-1} m_t \tag{26}$$

$$\theta_{t+1} \in \operatorname{prox}_{\alpha_t \rho_{\lambda}(\cdot; a)}^{C_t + \delta I}(\widehat{\theta}_t)$$
 (27)

$$= \underset{\theta}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\theta - \widehat{\theta}_t\|_{C_t + \delta I}^2 + \alpha_t \rho_{\lambda}(\theta; a) \right\}$$
 (28)

Since the program is coordinate-wise decomposable, we have for each coordinate

$$\theta_{t+1,i} = \begin{cases} \operatorname{sign}(\widehat{\theta}_{t,i}) \max\{|\widehat{\theta}_{t,i} - \widehat{\lambda}_i|, 0\} & \text{if } |\widehat{\theta}_{t,i}| \le 2\widehat{\lambda}_i \\ \frac{(a-1)\widehat{\theta}_{t,i} - \operatorname{sign}(\widehat{\beta}\theta_{t,i}a\widehat{\lambda}_i)}{a-2} & \text{if } 2\widehat{\lambda}_i < |\widehat{\theta}_{t,i}| \le a\widehat{\lambda}_i \\ \widehat{\theta}_{t,i} & \text{if } |\widehat{\theta}_{t,i}| > a\widehat{\lambda}_i \end{cases}$$
(29)

where $\widehat{\lambda}_i = \frac{\alpha_t \lambda}{C_{t,i} + \delta}$.

Although the derivations look little complicated for both cases, we emphasize that both two closed-form solutions can be efficiently implemented in a GPU-friendly manner.

Algorithm 2 PROXGENW: A General Stochastic Proximal Gradient Method with Weight Decay

- 1: **Input:** Stepsize α_t , $\{\rho_t\}_{t=1}^{t=T} \in [0,1)$, regularization parameter λ , small constant $0 < \delta \ll 1$, and weight decay regularization parameter ζ .
- 2: Initialize: $\theta_1 \in \mathbb{R}^d$, $m_0 = 0$, and $C_0 = 0$.
- 3: **for** $t = 1, 2, \dots, T$ **do**
- 4: Draw a minibatch sample ξ_t from \mathbb{P}
- 5: $g_t \leftarrow \nabla f(\theta_t; \xi_t)$

 \triangleright Stochastic gradient at time t

6: $m_t \leftarrow \rho_t m_{t-1} + (1 - \rho_t) g_t$

⊳ First-order momentum estimate

- 7: $C_t \leftarrow \text{Preconditioner construction}$
- 8: $\bar{\theta}_t \leftarrow (1 \alpha_t \zeta) \theta_t$

- ▷ Apply decoupled weight decay
- 9: $\theta_{t+1} \in \underset{\theta \in \Omega}{\operatorname{argmin}} \left\{ \langle m_t, \theta \rangle + \lambda \mathcal{R}(\theta) + \frac{1}{2\alpha_t} (\theta \bar{\theta}_t)^{\mathsf{T}} \left(C_t + \delta I \right) (\theta \bar{\theta}_t) \right\}$
- 10: **end for**
- 11: Output: θ_T

D Examples Satisfying Condition (C-4)

Theorem 2 (Weyl). For any two $n \times n$ Hermitian matrices A and B, assume that the eigenvalues of A and B are

$$\mu_1 \ge \cdots \ge \mu_n$$
, and $\nu_1 \ge \cdots \ge \nu_n$

respectively. Let $\lambda_1 \ge \cdots \ge \lambda_n$ be the eigenvalues of the matrix A + B, then the following holds

$$\mu_j + \nu_k \le \lambda_i \le \mu_r + \nu_s$$

for $j + k - n \ge i \ge r + s - 1$. Hence, we could derive

$$\lambda_1 \le \mu_1 + \nu_1$$

We provide concrete examples and derivations satisfying Condition (C-4) in Section 3.

Vanilla SGD. The vanilla SGD corresponds to $C_t = I$. We assume the constant stepsize $\alpha_t = \alpha$. Then, the condition (C-4) can be computed as

$$\lambda_{\min}(\alpha_t(C_t + \delta I)^{-1}) = \lambda_{\min}(\alpha \frac{1}{\delta + 1}I) = \frac{\alpha}{\delta + 1}$$

Therefore, we conclude that $\gamma = \frac{\alpha}{\delta + 1}$.

ADAGRAD. In PROXGEN framework, ADAGRAD corresponds to $C_t = \left(\frac{1}{t}\sum_{\tau=1}^t g_\tau g_\tau^\mathsf{T}\right)^{1/2}$. Under the constant stepsizes $\alpha_t = \alpha$, we have

$$\lambda_{\max}(C_t) = \frac{1}{\sqrt{t}} \lambda_{\max} \left(\sum_{\tau=1}^t g_\tau g_\tau^\mathsf{T} \right)^{1/2}$$

$$\leq \frac{1}{\sqrt{t}} \left(\sum_{\tau=1}^t \lambda_{\max} (g_\tau g_\tau^\mathsf{T}) \right)^{1/2}$$

$$= \frac{1}{\sqrt{t}} \left(\sum_{\tau=1}^t \|g_\tau\|_2^2 \right)^{1/2}$$

$$\leq G$$

Hence, the Condition (C-4) can be satisfied as

$$\lambda_{\min}(\alpha_t(C_t + \delta I)^{-1}) \ge \frac{\alpha}{G + \delta} := \gamma$$

RMSPROP and ADAM. Exponential moving average (a.k.a. EMA) approaches correspond to $C_t = \left(\beta C_{t-1} + (1-\beta)g_tg_t^\mathsf{T}\right)^{1/2}$ where $\beta \in [0,1)$ and g_t denotes the stochastic gradient at time t. The usual RMSPROP and ADAM use diagonal approximations for $g_tg_t^\mathsf{T}$, but here we consider more general form (i.e. including general full matrix gradient outer-product) as introduce in Yun et al. (2019a). First, we derive the upper bound for maximum eigenvalue for the matrix C_t . The matrix C_t can be expressed by

$$C_{t} = (\beta C_{t-1} + (1 - \beta)g_{t}g_{t}^{\mathsf{T}})^{1/2}$$

$$= (\beta^{2}C_{t-2} + \beta(1 - \beta)g_{t-1}g_{t-1}^{\mathsf{T}} + (1 - \beta)g_{t}g_{t}^{\mathsf{T}})^{1/2}$$

$$= \cdots$$

$$= ((1 - \beta)\sum_{i=1}^{t} \beta^{t-i}g_{i}g_{i}^{\mathsf{T}})^{1/2}$$

We can derive the upper bound for maximum eigenvalue of C_t using Weyl's theorem (Theorem 2) by

$$\lambda_{\max}(C_t) = \lambda_{\max} \left((1 - \beta) \sum_{i=1}^t \beta^{t-i} g_i g_i^{\mathsf{T}} \right)^{1/2}$$

$$\leq \left((1 - \beta) \sum_{i=1}^t \beta^{t-i} \lambda_{\max} (g_i g_i^{\mathsf{T}}) \right)^{1/2}$$

$$\leq \left((1 - \beta) G^2 \sum_{i=1}^t \beta^{t-i} \right)^{1/2}$$

$$\leq G (1 - \beta^t)^{1/2} \leq G$$

Hence, we have $\lambda_{\max}(C_t + \delta I) \leq G + \delta$. Also, we have

$$\lambda_{\max}(C_t + \delta I) = \frac{1}{\lambda_{\min}((C_t + \delta I)^{-1})} \le \frac{1}{G + \delta}$$

Therefore, the condition (C-4) under the constant stepsize $\alpha_t = \alpha$ can be derived as

$$\lambda_{\min} (\alpha_t (C_t + \delta I)^{-1}) \ge \frac{\alpha}{G + \delta}$$

which yields $\gamma = \frac{\alpha}{G + \delta}$.

Natural Gradient Descent. In this case, we derive the condition (C-4) for the Fisher information matrix when the loss function is defined as a negative log-likelihood, i.e., $f = \log p(x|\theta)$. The natural gradient descent aims at considering general geometry (not limited to Euclidean geometry), but we restrict our focus on the distribution space where the Fisher information is employed for preconditioner matrix C_t . The Fisher information matrix is defined as

$$F = \mathbb{E}_{Q(x)P(y|x,\theta)} \left[\frac{\partial f(x|\theta)}{\partial \theta} \frac{\partial f(x|\theta)}{\partial \theta}^{\mathsf{T}} \right]$$

where Q(x) is data distribution and $P(y|x,\theta)$ denotes the model's predictive distribution (ex. neural networks). However, in general, we do not have access to true data distribution, so we instead take an expectation with respect to empirical (training) data distribution $\widehat{Q}(x)$. This trick is also employed for K-FAC approximations to the Fisher Martens & Grosse (2015). Let the training samples be $\mathcal{S} = \{x_1, \cdots, x_n\}$ with sample size n. Then, the empirical Fisher could be computed as

$$\widehat{F} = \mathbb{E}_{\widehat{Q}(x)P(y|x,\theta)} \left[\frac{\partial f(x|\theta)}{\partial \theta} \frac{\partial f(x|\theta)}{\partial \theta}^{\mathsf{T}} \right]$$
$$= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial f(x_i|\theta)}{\partial \theta} \frac{\partial f(x_i|\theta)}{\partial \theta}^{\mathsf{T}}$$

Now, we bound the maximum eigenvalue of \hat{F} as

$$\lambda_{\max}(\widehat{F}) = \frac{1}{n} \sum_{i=1}^{t} \lambda_{\max} \left(\frac{\partial f(x_i | \theta)}{\partial \theta} \frac{\partial f(x_i | \theta)}{\partial \theta}^{\mathsf{T}} \right)$$

$$\leq \frac{1}{n} \sum_{i=1}^{t} G^2$$

$$= G^2$$

by our Condition (C-3). Hence, the Condition (C-4) can be derived as

$$\lambda_{\min}(\alpha_t(\widehat{F} + \delta I)^{-1}) \ge \frac{\alpha}{G^2 + \delta}$$

under the constant stepsize $\alpha_t = \alpha$.

E Proofs of Theorem 1

Lemma 1. The first-order momentum m_t in Algorithm 1 satisfies

$$||m_t||_2 \leq G$$

Proof. We use mathematical induction. For t=1, the momentum is computed as $m_1=\rho_1m_0+(1-\rho_1)g_t=(1-\rho_0)g_1$. Therefore, we have $\|m_t\|_2=\|(1-\rho_0)g_1\|\leq (1-\rho_0)G\leq G$.

Now, we assume that $||m_{t-1}||_2 \le G$ holds. The momentum at time t is constructed by $m_t = (1 - \rho_t)m_{t-1} + \rho_t g_t$. Then, we have

$$||m_t||_2 = ||(1 - \rho_t)m_{t-1} + \rho_t g_t||_2$$

$$\leq (1 - \rho_t)||m_{t-1}||_2 + \rho_t||g_t||_2$$

$$\leq (1 - \rho_t)G + \rho_t G = G$$

where the first inequality comes from the triangle inequality and the second one is derived from the induction hypothesis.

We deal with the following update rule in Algorithm 1 as

$$\theta_{t+1} \in \underset{\theta \in \Omega}{\operatorname{argmin}} \left\{ \left\langle (1 - \rho_t) g_t + \rho_t m_{t-1}, \theta \right\rangle + \mathcal{R}(\theta) + \frac{1}{2\alpha_t} (\theta - \theta_t)^\mathsf{T} (C_t + \delta I) (\theta - \theta_t) \right\}$$
(30)

By the optimality condition, we have

$$0 \in (1 - \rho_t)g_t + \rho_t m_{t-1} + \widehat{\partial} \mathcal{R}(\theta_{t+1}) + \frac{1}{\alpha_t} (C_t + \delta I)(\theta_{t+1} - \theta_t)$$

which means that

$$-(1-\rho_t)g_t - \rho_t m_{t-1} - \frac{1}{\alpha_t} (C_t + \delta I)(\theta_{t+1} - \theta_t) \in \widehat{\partial} \mathcal{R}(\theta_{t+1})$$

By adding the gradient $\nabla f(\theta_{t+1})$ on both sides, we have

$$\nabla f(\theta_{t+1}) - (1 - \rho_t)g_t - \rho_t m_{t-1} - \frac{1}{\alpha_t} (C_t + \delta I)(\theta_{t+1} - \theta_t) \in \nabla f(\theta_{t+1}) + \widehat{\partial} \mathcal{R}(\theta_{t+1}) = \widehat{\partial} F(\theta_{t+1})$$

By the definition of θ_{t+1} in Eq. (30), we obtain

$$\langle (1 - \rho_t)g_t + \rho_t m_{t-1}, \theta_{t+1} \rangle + \mathcal{R}(\theta_{t+1}) + \frac{1}{2\alpha_t} (\theta_{t+1} - \theta_t)^\mathsf{T} (C_t + \delta I)(\theta_{t+1} - \theta_t)$$

$$\leq \langle (1 - \rho_t)g_t + \rho_t m_{t-1}, \theta_t \rangle + \mathcal{R}(\theta_t)$$

which in result

$$\langle (1 - \rho_t)g_t + \rho_t m_{t-1}, \theta_{t+1} - \theta_t \rangle + \mathcal{R}(\theta_{t+1}) + \frac{1}{2\alpha_t} (\theta_{t+1} - \theta_t)^\mathsf{T} (C_t + \delta I)(\theta_{t+1} - \theta_t) \le \mathcal{R}(\theta_t)$$

Since the function f is L-smooth by Condition (C-1), we have

$$f(\theta_{t+1}) \le f(\theta_t) + \langle \nabla f(\theta_t), \theta_{t+1} - \theta_t \rangle + \frac{L}{2} \|\theta_{t+1} - \theta_t\|_2^2$$

Adding previous two inequalities yields

$$\langle (1 - \rho_t)g_t - \nabla f(\theta_t) + \rho_t m_{t-1}, \theta_{t+1} - \theta_t \rangle + (\theta_{t+1} - \theta_t)^\mathsf{T} \left(\frac{1}{2\alpha_t} (C_t + \delta I) - \frac{L}{2} I \right) (\theta_{t+1} - \theta_t)$$

$$\leq F(\theta_t) - F(\theta_{t+1}) \tag{31}$$

Then, we have

$$\begin{aligned} &\|\theta_{t+1} - \theta_{t}\|_{\frac{1}{2\alpha_{t}}(C_{t} + \delta I) - \frac{L}{2}I}^{2} \\ &\stackrel{\bigcirc}{\leq} F(\theta_{t}) - F(\theta_{t+1}) - \left\langle (1 - \rho_{t})g_{t} - \nabla f(\theta_{t}), \theta_{t+1} - \theta_{t} \right\rangle - \left\langle \rho_{t} m_{t-1}, \theta_{t+1} - \theta_{t} \right\rangle \\ &= F(\theta_{t}) - F(\theta_{t+1}) - \left\langle g_{t} - \nabla f(\theta_{t}), \theta_{t+1} - \theta_{t} \right\rangle + \left\langle \rho_{t} g_{t}, \theta_{t+1} - \theta_{t} \right\rangle - \left\langle \rho_{t} m_{t-1}, \theta_{t+1} - \theta_{t} \right\rangle \\ &\stackrel{\bigcirc}{\leq} F(\theta_{t}) - F(\theta_{t+1}) + \frac{1}{2L} \|g_{t} - \nabla f(\theta_{t})\|_{2}^{2} + \frac{L}{2} \|\theta_{t+1} - \theta_{t}\|_{2}^{2} + \frac{\rho_{t}^{2}}{2L} \|g_{t}\|_{2}^{2} + \frac{L}{2} \|\theta_{t+1} - \theta_{t}\|_{2}^{2} \\ &+ \|\rho_{t} m_{t-1}\|_{2} \|\theta_{t+1} - \theta_{t}\|_{2} \end{aligned}$$

$$\stackrel{\bigcirc}{\leq} F(\theta_{t}) - F(\theta_{t+1}) + \rho_{0} \mu^{t-1} DG + \frac{\rho_{0}^{2} \mu^{2(t-1)} G^{2}}{2L} + L \|\theta_{t+1} - \theta_{t}\|_{2}^{2} + \frac{1}{2L} \|g_{t} - \nabla f(\theta_{t})\|_{2}^{2} \end{aligned}$$

The derivations in inequalities (1-3) as follows:

- 1) We rearrange the inequality Eq. (31).
- ② We use the fact that $\langle a,b\rangle \leq \frac{1}{2}\|a\|_2^2 + \frac{1}{2}\|b\|_2^2$ and $\langle a,b\rangle \leq \|a\|_2\|b\|_2$. With this, we use modified version such as $\langle a,b\rangle = \langle ca,\frac{1}{c}b\rangle \leq c^2\|a\|_2^2 + \frac{1}{c^2}\|b\|_2^2$ for any positive constant c.
- (3) We apply our Lemma 1 and Condition (C-3).

By rearranging the above inequality, we require the following quantity be positive-semidefinite.

$$\frac{1}{2\alpha_t}(C_t + \delta I) - \frac{3}{2}LI \succeq 0$$

Note that in this inequality we can see that

$$\frac{1}{2\alpha_t}(C_t + \delta I) - \frac{3}{2}LI \succeq \frac{1}{2\alpha_0}\delta I - \frac{3}{2}LI$$

since C_t is positive (semi)definite and α_t is *non-increasing*. Therefore, from this we can derive the stepsize condition in our Theorem 1 as

$$\alpha_0 \le \frac{\delta}{3L}$$

Therefore, we have

$$\sum_{t=0}^{T-1} \|\theta_{t+1} - \theta_t\|_{\frac{1}{2\alpha_t}(C_t + \delta I) - \frac{3}{2}LI}^2 \leq \underbrace{F(\theta_0) - F(\theta^*)}_{\Delta} + \underbrace{\frac{\rho_0 DG}{1 - \mu} + \frac{\rho_0^2 G^2}{2L(1 - \mu^2)}}_{C_1} + \frac{1}{2L} \sum_{t=0}^{T-1} \|g_t - \nabla f(\theta_t)\|_2^2$$

$$\leq \Delta + C_1 + \frac{1}{2L} \sum_{t=0}^{T-1} \|g_t - \nabla f(\theta_t)\|_2^2$$

Furthermore, we also have by stepsize condition

$$\left(\frac{\delta}{2\alpha_0} - \frac{3}{2}L\right) \sum_{t=0}^{T-1} \|\theta_{t+1} - \theta_t\|_2^2 \le \sum_{t=0}^{T-1} \|\theta_{t+1} - \theta_t\|_{\frac{1}{2\alpha_t}(C_t + \delta I) - \frac{3}{2}LI}^2 \le \Delta + C_1 + \frac{1}{2L} \sum_{t=0}^{T-1} \|g_t - \nabla f(\theta_t)\|_2^2$$

since $\delta I \leq C_t + \delta I$. From above inequality, we obtain

$$\sum_{t=0}^{T-1} \|\theta_{t+1} - \theta_t\|_2^2 \le H_1 + H_2 \sum_{t=0}^{T-1} \|g_t - \nabla f(\theta_t)\|_2^2$$
(32)

where the constants H_1 and H_2 are defined as

$$H_1 = \Delta / \left(\frac{\delta}{2\alpha_0} - \frac{3}{2}L\right) + C_1 / \left(\frac{\delta}{2\alpha_0} - \frac{3}{2}L\right)$$

$$H_2 = \frac{1}{2L(\frac{\delta}{2\alpha_0} - \frac{3}{2}L)}$$

Our goal is to bound the distance between the zero vector and subdifferential set of F, so we have

$$\begin{aligned}
&\operatorname{dist}(\mathbf{0}, \widehat{\partial}F(\theta_{t+1}))^{2} \\
&= \left\| (1 - \rho_{t})g_{t} - \nabla f(\theta_{t+1}) + \rho_{t}m_{t-1} + \frac{1}{\alpha_{t}}(C_{t} + \delta I)(\theta_{t+1} - \theta_{t}) \right\|_{2}^{2} \\
&= \left\| (1 - \rho_{t})g_{t} - \nabla f(\theta_{t+1}) + \rho_{t}m_{t-1} + (\theta_{t+1} - \theta_{t}) + \frac{1}{\alpha_{t}}(C_{t} + \delta I)(\theta_{t+1} - \theta_{t}) - (\theta_{t+1} - \theta_{t}) \right\|_{2}^{2} \\
&\leq 3 \left\| (1 - \rho_{t})g_{t} - \nabla f(\theta_{t+1}) + \rho_{t}m_{t-1} + (\theta_{t+1} - \theta_{t}) \right\|_{2}^{2} \\
&+ 3 \left\| \frac{1}{\alpha_{t}}(C_{t} + \delta I)(\theta_{t+1} - \theta_{t}) \right\|_{2}^{2} + 3 \left\| (\theta_{t+1} - \theta_{t}) \right\|_{2}^{2} \\
&\leq 3 \underbrace{\left\| (1 - \rho_{t})g_{t} - \nabla f(\theta_{t+1}) + \rho_{t}m_{t-1} + (\theta_{t+1} - \theta_{t}) \right\|_{2}^{2}}_{T_{1}} + 3 \left(\frac{1}{\gamma^{2}} + 1 \right) \|\theta_{t+1} - \theta_{t}\|_{2}^{2}
\end{aligned}$$

Here, we assume that

$$\lambda_{\max} \left(\frac{1}{\alpha_t} (C_t + \delta I) \right) \le \frac{1}{\gamma}$$

which yields our Condition (C-4)

$$\lambda_{\min} \left(\alpha_t (C_t + \delta I)^{-1} \right) \ge \gamma$$

From Eq. (31), we have

$$\langle (1 - \rho_t)g_t - \nabla f(\theta_t) + \rho_t m_{t-1}, \theta_{t+1} - \theta_t \rangle + \|\theta_{t+1} - \theta_t\|_{\frac{1}{2\alpha_t}(C_t + \delta I) - \frac{L}{2}I}^2 \le F(\theta_t) - F(\theta_{t+1})$$

which can be re-written as

$$\left\langle (1 - \rho_t)g_t - \nabla f(\theta_{t+1}) + \rho_t m_{t-1}, \theta_{t+1} - \theta_t \right\rangle$$

$$\leq F(\theta_t) - F(\theta_{t+1}) - \left\langle \nabla f(\theta_{t+1}) - \nabla f(\theta_t), \theta_{t+1} - \theta_t \right\rangle - \left\| \theta_{t+1} - \theta_t \right\|_{\frac{1}{2\alpha_t}(C_t + \delta I) - \frac{L}{2}I}^2$$

$$\leq F(\theta_t) - F(\theta_{t+1}) - \left\langle \nabla f(\theta_{t+1}) - \nabla f(\theta_t), \theta_{t+1} - \theta_t \right\rangle + \left(\frac{\delta}{2\alpha_0} - \frac{L}{2}\right) \|\theta_{t+1} - \theta_t\|_2^2$$

since we have the condition $\frac{\delta}{2\alpha_0} \geq \frac{3}{2}L$. Therefore, we obtain

$$T_{1} = \|(1 - \rho_{t})g_{t} - \nabla f(\theta_{t+1}) + \rho_{t}m_{t-1}\|_{2}^{2} + \|\theta_{t+1} - \theta_{t}\|_{2}^{2}$$

$$+ 2\left\langle (1 - \rho_{t})g_{t} - \nabla f(\theta_{t+1}) + \rho_{t}m_{t-1}, \theta_{t+1} - \theta_{t} \right\rangle$$

$$\leq \|(1 - \rho_{t})g_{t} - \nabla f(\theta_{t}) + \nabla f(\theta_{t}) - \nabla f(\theta_{t+1}) + \rho_{t}m_{t-1}\|_{2}^{2} + \|\theta_{t+1} - \theta_{t}\|_{2}^{2}$$

$$+ F(\theta_{t}) - F(\theta_{t+1}) - \left\langle \nabla f(\theta_{t+1}) - \nabla f(\theta_{t}), \theta_{t+1} - \theta_{t} \right\rangle + \left(\frac{\delta}{2\alpha_{0}} - \frac{L}{2}\right) \|\theta_{t+1} - \theta_{t}\|_{2}^{2}$$

$$\leq 4\|g_{t} - \nabla f(\theta_{t})\|_{2}^{2} + 4L^{2}\|\theta_{t+1} - \theta_{t}\|_{2}^{2} + 4\|\rho_{t}m_{t-1}\|_{2}^{2} + 4\|\rho_{t}g_{t}\|_{2}^{2} + \|\theta_{t+1} - \theta_{t}\|_{2}^{2}$$

$$+ F(\theta_{t}) - F(\theta_{t+1}) + L\|\theta_{t+1} - \theta_{t}\|_{2}^{2} + \left(\frac{\delta}{2\alpha_{0}} - \frac{L}{2}\right) \|\theta_{t+1} - \theta_{t}\|_{2}^{2}$$

$$\leq F(\theta_{t}) - F(\theta_{t+1}) + 4\rho_{0}^{2}\mu^{2(t-1)}G^{2} + 4\rho_{0}^{2}\mu^{2(t-1)}G^{2}$$

$$+ \left(\frac{\delta}{2\alpha_{0}} + \frac{L}{2} + 1 + 4L^{2}\right) \|\theta_{t+1} - \theta_{t}\|_{2}^{2} + 4\|g_{t} - \nabla f(\theta_{t})\|_{2}^{2}$$

Therefore, we have the distance as

$$\operatorname{dist}(\mathbf{0}, \widehat{\partial} F(\theta_{t+1}))^{2} \leq 3 \left(F(\theta_{t}) - F(\theta_{t+1}) + 8\rho_{0}^{2} \mu^{2(t-1)} G^{2} + \left(\underbrace{\frac{\delta}{2\alpha_{0}} + \frac{L}{2} + 2 + 4L^{2} + \frac{1}{\gamma^{2}}}_{C_{2}} \right) \|\theta_{t+1} - \theta_{t}\|_{2}^{2} + 4\|g_{t} - \nabla f(\theta_{t})\|_{2}^{2} \right)$$

Therefore, we have

$$\mathbb{E}[\operatorname{dist}(\mathbf{0}, \widehat{\partial} F(\theta_{a}))^{2}] \leq \frac{1}{T} \sum_{t=0}^{T-1} \mathbb{E}\Big[\| (1 - \rho_{t}) g_{t} - \nabla f(\theta_{t+1}) + \rho_{t} m_{t-1} + \frac{1}{\alpha_{t}} (C_{t} + \delta I) (\theta_{t+1} - \theta_{t}) \|_{2}^{2} \Big]$$

$$\leq \frac{3}{T} \Big(\Delta + \frac{8\rho_{0}^{2} G^{2}}{1 - \mu^{2}} + 4 \sum_{t=0}^{T-1} \| g_{t} - \nabla f(\theta_{t}) \|_{2}^{2} + C_{2} \sum_{t=0}^{T-1} \| \theta_{t+1} - \theta_{t} \|_{2}^{2} \Big)$$

$$\leq \frac{3}{T} \Big(\Delta + \frac{8\rho_{0}^{2} G^{2}}{1 - \mu^{2}} + 4 \sum_{t=0}^{T-1} \| g_{t} - \nabla f(\theta_{t}) \|_{2}^{2} + C_{2} (H_{1} + H_{2} \sum_{t=0}^{T-1} \| g_{t} - \nabla f(\theta_{t}) \|_{2}^{2} \Big)$$

$$\leq \frac{Q_{1}}{T} \sum_{t=0}^{T-1} \mathbb{E} \Big[\| g_{t} - \nabla f(\theta_{t}) \|_{2}^{2} \Big] + \frac{Q_{2} \Delta}{T} + \frac{Q_{3}}{T}$$

where

$$Q_1 = 4 + C_2 H_2$$
, $Q_2 = 3 + \frac{3C_2}{\frac{\delta}{2\alpha_0} - \frac{3}{2}L}$, $Q_3 = \frac{24\rho_0^2 G^2}{1 - \mu^2} + \frac{3C_1 C_2}{\frac{\delta}{2\alpha_0} - \frac{3}{2}L}$

Note that the constants Q_1 , Q_2 , and Q_3 depend on $\{\alpha_0, \delta, L, D, G, \rho_0, \mu, \gamma\}$, but not on T. The third inequality comes from Eq. (32). If we assume the stochastic gradient g_t is evaluated on the minibatch S_t with $|S_t| = b_t$, then we can obtain using Condition (C-2)

$$||g_{t} - \nabla f(\theta_{t})||_{2}^{2} = \mathbb{E}_{\xi} \left[\left\| \frac{1}{b_{t}} \sum_{i=1}^{b_{t}} \nabla f(\theta_{t}; \xi_{i_{t}}) - \nabla f(\theta_{t}) \right\|_{2}^{2} \right]$$

$$= \frac{1}{b_{t}^{2}} \mathbb{E} \left[\left\| \sum_{i=1}^{b_{t}} \left\{ \nabla f(\theta_{t}; \xi_{i_{t}}) - \nabla f(\theta_{t}) \right\} \right\|_{2}^{2} \right]$$

$$\leq \frac{1}{b_{t}^{2}} \sum_{i_{t}=1}^{b_{t}} \mathbb{E} \left[\left\| \nabla f(\theta_{t}; \xi_{i_{t}}) - \nabla f(\theta_{t}) \right\|_{2}^{2} \right] \leq \frac{1}{b_{t}} \sigma^{2}$$

where i_t represents the random variable for each datapoint in minibatch samples S_t . Finally, we arrive at our Theorem 1 as

$$\mathbb{E}_{R}[\operatorname{dist}(\mathbf{0},\widehat{\partial}F(\theta_{R}))^{2}] \leq \frac{Q_{1}\sigma^{2}}{T} \sum_{t=0}^{T-1} \frac{1}{b_{t}} + \frac{Q_{2}\Delta}{T} + \frac{Q_{3}}{T}$$