

BILEVEL OPTIMIZATION WITH CONVEX MAJORANT APPROACH FOR TRAINING SPARSE NEURAL NETWORKS

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Abstract. This paper proposes a convex majorant approach for training sparse neural networks by bilevel optimization where the upper level problem minimizes a smooth nonconvex function while the lower level problem minimizes a smooth nonconvex function with a nonsmooth convex group sparse regularizer over a box set for fixed sparse regularization hyperparameters. The convex majorant function approximates the objective function of the lower level problem. We establish the relationship between the original bilevel optimization and the bilevel optimization with the convex majorant approach regarding global and local minimizers. Moreover, we use a smoothing function to approximate the convex majorant function, and derive the convergence of global minimizers to those of the corresponding nonsmooth bilevel problems with smoothing parameter converging to zero. A smoothing implicit function method is proposed to solve the smooth approximate bilevel optimization problem. Some numerical experiments including the tests on the data from machine learning repository show that the convex majorant approach performs better than the widely used Grid Search method, Random Search method and Bayesian optimization method.

Key words. Bilevel optimization, sparse regularization hyperparameter, convex majorant, smoothing method

AMS subject classifications. 90C30, 90C33, 90C90

1. Introduction. In this paper, we consider bilevel optimization for tuning hyperparameters of L -layer sparse feed-forward neural networks with L being a positive integer. We divide the given data $\{(X^i, Y^i) \in \mathbb{R}^n \times \mathbb{R}^m, i = 1, \dots, N\}$ into a training set $\{(X^i, Y^i) \in \mathbb{R}^n \times \mathbb{R}^m, i = 1, \dots, N_{tr}\}$ and a validation set $\{(X^i, Y^i) \in \mathbb{R}^n \times \mathbb{R}^m, i = N_{tr} + 1, \dots, N\}$, where $N = N_{tr} + N_{va}$. Let $W_\ell \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$, $b^\ell \in \mathbb{R}^{n_\ell}$, $\alpha^\ell \in \mathbb{R}^{n_{\ell-1}}$ for $\ell = 1, \dots, L$, where $n_0 = n$ and $n_L = m$. The bilevel optimization involves the following functions:

$$\begin{aligned} F(u) &= \frac{1}{N_{va}} \sum_{i=N_{tr}+1}^N \|W_L \sigma(\dots \sigma(W_1 X^i + b^1) \dots) + b^L - Y^i\|^2, \\ H(u) &= \frac{1}{N_{tr}} \sum_{i=1}^{N_{tr}} \|W_L \sigma(\dots \sigma(W_1 X^i + b^1) \dots) + b^L - Y^i\|^2, \\ Q(w; \lambda) &= \sum_{\ell=1}^L \sum_{j=1}^{n_{\ell-1}} \alpha_j^\ell \|(W_\ell)_{\cdot j}\|, \end{aligned}$$

where $w = ((W_1)_{\cdot 1}^\top, \dots, (W_1)_{\cdot n}^\top, \dots, (W_L)_{\cdot n_{L-1}}^\top)^\top \in \mathbb{R}^p$, $b = ((b^1)^\top, \dots, (b^L)^\top)^\top \in \mathbb{R}^s$, $u = (w^\top, b^\top)^\top \in \mathbb{R}^q$, $\lambda = ((\alpha^1)^\top, \dots, (\alpha^L)^\top)^\top \in \mathbb{R}^r$ with $p = \sum_{\ell=1}^L n_{\ell-1} n_\ell$,

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30 $s = \sum_{\ell=1}^L n_\ell$, $r = \sum_{\ell=1}^L n_{\ell-1}$, $q = p + s$, and $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ is a twice continuously dif-
 31 ferentiable activation function. Here $\|\cdot\|$ denotes the Euclidean norm and $\sigma(u) :=$
 32 $(\sigma(u_1), \dots, \sigma(u_q))^\top$ for $u \in \mathbb{R}^q$. The functions F and H are smooth nonconvex,
 33 while the function $Q(\cdot; \lambda)$ is nonsmooth convex for any fixed sparse regularization
 34 hyperparameter $\lambda \geq 0$.

35 We focus on the following bilevel optimization problem:

$$36 \quad (1.1) \quad \min_{\lambda, u} F(u) \quad \text{s.t.} \quad \lambda \geq 0, \quad u \in S(\lambda),$$

37 where $S(\lambda)$ is the solution set of the lower level problem parameterized by λ :

$$38 \quad (1.2) \quad \min_u H(u) + Q(u; \lambda) \quad \text{s.t.} \quad u \in \Omega.$$

39 Here $\Omega := [\underline{u}, \bar{u}] \subseteq \mathbb{R}^q$ is a compact box set with $\underline{u} < \bar{u}$.

40 The feed-forward neural network is an important kind of neural networks. Ac-
 41 cording to the universal approximation theorem [2, 11, 23, 37], a feed-forward neural
 42 network with a single hidden layer can approximate any continuous function to any
 43 desired accuracy as long as the activation function is not polynomial and there are
 44 sufficient hidden nodes. In many applications, the sparse neural networks have ad-
 45 vantages for saving storage cost and computation cost [14, 40, 42]. Moreover, sparse
 46 neural networks have simpler structures and fewer parameters compared to the fully
 47 connected feed-forward neural networks, which can avoid data overfitting problems
 48 [13, 40].

49 The sparse regularization term $Q(u; \lambda)$ in (1.2) helps training the neural network
 50 with weight matrices W_ℓ , $\ell = 1, \dots, L$, that have few nonzero columns. This term is
 51 based on group sparse regularization which has been extensively employed in designing
 52 compact neural networks [14, 20, 38, 40, 42, 43]. Via this regularization technique,
 53 some columns of the weight matrices are forced to be zero simultaneously. Intuitively,
 54 this means that some connections of two neurons of two adjacent different levels are
 55 eliminated, which results in sparse neural networks (see [14, Figure 1] for an example).

56 There is no doubt that the selection of hyperparameters is crucial in constructing
 57 the sparse neural networks (see [38, Fig. 4]). In most related papers, the hyper-
 58 parameters are set via the Grid Search method [14, 38], which may not yield an
 59 optimal selection in general. A lot of evidences show that the bilevel optimization
 60 model is efficient and promising for hyperparameter selection in machine learning
 61 [15, 18, 28, 34, 35]. Hence, in this paper we study the nonsmooth nonconvex bilevel
 62 optimization (1.1) for the selection of optimal hyperparameters.

63 Since lower level problem (1.2) is nonsmooth and nonconvex, it is extremely chal-
 64 lenging to solve problem (1.1). One approach for bilevel optimization problems is to
 65 reformulate the bilevel optimization problem as a single level optimization problem
 66 with optimality conditions of the lower level optimization problem as constraints (see
 67 [12, Chapter 12]). However, it has been shown in [32, Example 1] and [33, Exam-
 68 ple 1.1] that when the lower level optimization problem is nonconvex, any optimal
 69 solution of the bilevel optimization problem may not even be a stationary point of
 70 the new single level optimization problem. Another method addressing nonconvex
 71 lower level problems is to use the value function, where the bilevel program is refor-
 72 mulated as a single level optimization problem via the value function, which can be
 73 solved via some existing algorithms for the nonconvex and nonsmooth optimization
 74 problems, see [24, 27, 41]. There are some other methods including the bounding

algorithm [33] and gradient method [29, 31]. Li and Yang [25] constructed a piecewise convex relaxation of the nonconvex lower level problem by adding a quadratic term. However, all of these works tend to be complicated and impractical for large-scale bilevel optimization problems. Moreover, the objective functions of the lower level problems in [24, 25, 27, 29, 31, 41] are assumed to be smooth, while problem (1.2) is nonsmooth. In [1, 34], the authors directly reformulated the bilevel optimization problems with nonsmooth and nonconvex lower level problems via optimality conditions of the lower level optimization problems, and employed smoothing methods to solve the resulting single level problems. In [30], the authors proposed a single-loop gradient-based algorithm by the Moreau envelope-based reformulation. However, as we have stated above, the equivalence between the original bilevel problem and the single level problem may fail due to the nonconvexity of the lower level problem.

We construct the following strongly convex majorant function with fixed $\lambda \in \mathbb{R}_+^r$, $z \in \Omega$ and $\gamma > 0$:

$$G(u; \lambda, z) := H(z) + \nabla H(z)^\top (u - z) + \frac{\gamma}{2} \|u - z\|^2 + Q(w; \lambda)$$

for $u \in \Omega$. Since H is twice continuously differentiable and Ω is a compact set, we can choose γ such that $\|\nabla^2 H(\cdot)\| \leq \gamma$ over Ω . The choice of γ guarantees that given any fixed $\lambda \in \mathbb{R}_+^r$, $z \in \Omega$,

$$G(u; \lambda, z) \geq H(u) + Q(w; \lambda)$$

for $u \in \Omega$. Now we consider the following problem:

$$(1.3) \quad \min_{\lambda, z, u} F(u) \quad \text{s.t.} \quad \lambda \geq 0, \quad z \in \Omega, \quad u = u(\lambda, z),$$

where $u(\lambda, z)$ is the unique solution of the following lower level problem:

$$(1.4) \quad \min_u G(u; \lambda, z) \quad \text{s.t.} \quad u \in \Omega.$$

The convex majorant approach (1.4) is based on the second order Taylor expansion, which is different from the piecewise convex relaxation in [25]. Note that although the objective function $G(\cdot; \lambda, z)$ of problem (1.4) is nonsmooth, it can have a smoothing function with the gradient consistency (see [7] for the definition). In particular, we propose a strongly convex smoothing function

$$(1.5) \quad G_\mu(u; \lambda, z) := H(z) + \nabla H(z)^\top (u - z) + \frac{\gamma}{2} \|u - z\|^2 + Q_\mu(w; \lambda)$$

for $u \in \Omega$, where $\mu > 0$ is an arbitrarily small real number and

$$(1.6) \quad Q_\mu(w; \lambda) = \sum_{\ell=1}^L \sum_{j=1}^{n_{\ell-1}} \alpha_j^\ell \sqrt{\|(W_\ell)_{\cdot j}\|^2 + \mu}.$$

For any fixed λ and z , we have

$$(1.7) \quad \lim_{u \rightarrow \tilde{u}, \mu \downarrow 0} G_\mu(u; \lambda, z) = G(\tilde{u}; \lambda, z) \quad \text{and} \quad \text{conv} \left\{ \lim_{u \rightarrow \tilde{u}, \mu \downarrow 0} \nabla G_\mu(u; \lambda, z) \right\} = \partial G(\tilde{u}; \lambda, z),$$

where conv denotes the convex hull and $\partial G(\tilde{u}; \lambda, z)$ is the Clarke subgradient of G at \tilde{u} [9].

The contributions of this paper are summarized as follows.

(i) We propose a convex majorant approach (1.3) for problem (1.1) by replacing the objective function of the lower level problem (1.2) with a convex majorant function $G(\cdot; \lambda, z)$. We then derive the equivalence between the global and local optimal solutions of problem (1.1) and problem (1.3) under the assumptions on feasibility.

(ii) We use the smoothing function $G_\mu(\cdot; \lambda, z)$ to define a smooth approximation problem of problem (1.3). We prove that any accumulation point of global optimal solutions of the smooth approximation problems is the global optimal solution of problem (1.3) as the smoothing parameter μ goes to zero.

(iii) We propose a smoothing implicit function method to solve the smooth approximate problem of problem (1.3), and derive the convergence of the method to a Clarke stationary point of the smooth approximate problem.

This paper is organized as follows. In Section 2, we establish the relationship between problem (1.1) and problem (1.3) regarding global and local optimal solutions. We study the smooth approximation problem of problem (1.3) in Section 3. In Section 4, we propose a smoothing implicit function method. Numerical results are presented in Section 5. Finally, concluding remarks are drawn in Section 6.

Notation: Denote a closed ball in \mathbb{R}^q with center $u \in \mathbb{R}^q$ and radius $\delta > 0$ by $B(u, \delta)$. Let I_q be the identity matrix in $\mathbb{R}^{q \times q}$, and $e_q \in \mathbb{R}^q$ be the vector with all elements equal to 1. Given function $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$, $Jf(x) \in \mathbb{R}^{n \times m}$ denotes the Jacobian of f at $x \in \mathbb{R}^m$. Let $\text{diag}(v) \in \mathbb{R}^{q \times q}$ be the square matrix with elements of $v \in \mathbb{R}^q$ on the diagonal. Given a nonempty closed convex set $S \subset \mathbb{R}^q$, $N_S(x) := \{v : \langle v, y - x \rangle \leq 0, \forall y \in S\}$ denotes the normal cone of S at x .

2. Relationship between problems (1.1) and (1.3). In this section, we investigate the relationship between problem (1.1) and problem (1.3). We assume that the solution sets of problems (1.1) and (1.3) are nonempty. The following lemma indicates the relationship in regard to the feasibility. As for problem (1.1), $(\tilde{\lambda}, \tilde{u})$ is a feasible point of problem (1.1) if $\tilde{\lambda} \geq 0$, $\tilde{u} \in \Omega$, and \tilde{u} solves lower level problem (1.2) globally for the fixed hyperparameter $\tilde{\lambda}$. The feasibility of problem (1.3) can be defined similarly.

LEMMA 2.1. *If $(\tilde{\lambda}, \tilde{u})$ is a feasible point of problem (1.1), then $(\tilde{\lambda}, \tilde{u}, \tilde{u})$ is a feasible point of problem (1.3).*

Proof. It suffices to prove that $G(\tilde{u}; \tilde{\lambda}, \tilde{u}) \leq G(u; \tilde{\lambda}, \tilde{u})$ for any $u \in \Omega$. Note that

$$G(\tilde{u}; \tilde{\lambda}, \tilde{u}) = H(\tilde{u}) + Q(\tilde{u}; \tilde{\lambda}) \leq H(u) + Q(u; \tilde{\lambda}) \leq G(u; \tilde{\lambda}, \tilde{u}),$$

since $\tilde{u} \in S(\tilde{\lambda})$. The conclusion is obvious. \square

From Lemma 2.1, the following two theorems give some properties of global and local optimal solutions of problem (1.3) related to problem (1.1).

THEOREM 2.2. *Let $(\tilde{\lambda}, \tilde{z}, \tilde{u})$ be a global optimal solution of problem (1.3). Then the following statements hold.*

(i) $F(\tilde{u}) \leq F(u)$, for any feasible point $u \in S(\tilde{\lambda})$, $\tilde{\lambda} \geq 0$ of problem (1.1).

(ii) If $(\tilde{\lambda}, \tilde{u})$ is a feasible point for problem (1.1), then $(\tilde{\lambda}, \tilde{u})$ is a global optimal solution of (1.1).

Proof. (i) According to Lemma 2.1, for any feasible point $u \in S(\tilde{\lambda})$, $\tilde{\lambda} \geq 0$ of problem (1.1), $(\tilde{\lambda}, u, u)$ is a feasible point of problem (1.3). Since $(\tilde{\lambda}, \tilde{z}, \tilde{u})$ is a global optimal solution of problem (1.3), we have $F(\tilde{u}) \leq F(u)$.

(ii) Assume by contradiction that $(\tilde{\lambda}, \tilde{u})$ is not a global optimal solution of (1.1). Then there exists a feasible point (λ^*, u^*) of problem (1.1) such that $F(u^*) < F(\tilde{u})$. Due to Lemma 2.1, we know that (λ^*, u^*, u^*) is a feasible point of problem (1.3).

However, the fact that $F(u^*) < F(\tilde{u})$ contradicts the hypothesis that $(\tilde{\lambda}, \tilde{z}, \tilde{u})$ is a global optimal solution of (1.3). \square

THEOREM 2.3. *Let $(\tilde{\lambda}, \tilde{u}, \tilde{u})$ be a local optimal solution of problem (1.3). If $(\tilde{\lambda}, \tilde{u})$ is a feasible point of problem (1.1), then $(\tilde{\lambda}, \tilde{u})$ is a local optimal solution of problem (1.1).*

Proof. Assume by contradiction that $(\tilde{\lambda}, \tilde{u})$ is not a local optimal solution of problem (1.1). Then there exists a sequence of feasible points (λ^k, u^k) , $k = 1, 2, \dots$, of problem (1.1) satisfying that

$$\lim_{k \rightarrow \infty} (\lambda^k, u^k) = (\tilde{\lambda}, \tilde{u}), \text{ and } F(u^k) < F(\tilde{u}), \text{ } k = 1, 2, \dots.$$

Based on Lemma 2.1, we know that (λ^k, u^k, u^k) , $k = 1, 2, \dots$, are feasible points of problem (1.3). Hence, for any neighborhood of $(\tilde{\lambda}, \tilde{u}, \tilde{u})$, we can find some (λ^k, u^k, u^k) in this neighborhood such that $F(u^k) < F(\tilde{u})$, which incurs a contradiction with the hypothesis that $(\tilde{\lambda}, \tilde{u}, \tilde{u})$ is a local optimal solution of problem (1.3). Thus we have proved that $(\tilde{\lambda}, \tilde{u})$ is a local optimal solution of problem (1.1). \square

Now we give a property of global optimal solutions of problem (1.1) related to problem (1.3).

THEOREM 2.4. *Let $(\tilde{\lambda}, \tilde{u})$ be a global (or local) optimal solution of (1.1). Then $(\tilde{\lambda}, \tilde{u}, \tilde{u})$ is a global (or local) optimal solution of (1.3) on $S_1 := \{(\lambda, u, u) : u \in S(\lambda), \lambda \geq 0\}$.*

Proof. We first prove the conclusion corresponding to the global optimal solution. Due to Lemma 2.1, it is obvious that $(\tilde{\lambda}, \tilde{u}, \tilde{u})$ is a feasible point of problem (1.3). According to the definition of S_1 , (λ^*, u^*) is a feasible point of problem (1.1) when $(\lambda^*, u^*, u^*) \in S_1$. Then we have $F(u^*) \geq F(\tilde{u})$ since $(\tilde{\lambda}, \tilde{u})$ is a global optimal solution of problem (1.1), which indicates that $(\tilde{\lambda}, \tilde{u}, \tilde{u})$ is a global optimal solution of problem (1.3) on S_1 . The conclusion corresponding to the local optimal solution can be proved like the proof for Theorem 2.3, which is omitted here. \square

In the following, we investigate properties of the solution function $u(\cdot, \cdot)$ of problem (1.4).

PROPOSITION 2.5. *The solution function $u : \mathbb{R}_+^r \times \Omega \rightarrow \mathbb{R}^q$ is Lipschitz continuous with Lipschitz constant $\kappa := \max\{2, \frac{\sqrt{r}}{\gamma}\}$, i.e., for any $(\lambda^1, z^1), (\lambda^2, z^2) \in \mathbb{R}_+^r \times \Omega$,*

$$(2.1) \quad \|u(\lambda^1, z^1) - u(\lambda^2, z^2)\| \leq \kappa(\|z^1 - z^2\| + \|\lambda^1 - \lambda^2\|).$$

Proof. Given $(\lambda^1, z^1), (\lambda^2, z^2) \in \mathbb{R}_+^r \times \Omega$, denote $u^1 := u(\lambda^1, z^1)$ and $u^2 := u(\lambda^2, z^2)$. According to the first order optimality condition, we have

$$\langle \nabla H(z^i) + \gamma(u^i - z^i) + \xi^i, z - u^i \rangle \geq 0, \quad \forall z \in \Omega, \quad i = 1, 2,$$

where $\xi^1 = ((\zeta^1)^\top, 0^\top)^\top \in \mathbb{R}^q$ with $\zeta^1 \in \partial Q(w^1; \lambda^1)$ and $\xi^2 = ((\zeta^2)^\top, 0^\top)^\top \in \mathbb{R}^q$ with $\zeta^2 \in \partial Q(w^2; \lambda^2)$. By setting $z = u^2$ and $z = u^1$ in the above two inequalities respectively and combining them, we have

$$\langle \nabla H(z^1) - \nabla H(z^2) + \gamma(u^1 - u^2) - \gamma(z^1 - z^2) + \xi^1 - \xi^2, u^2 - u^1 \rangle \geq 0,$$

which is equivalent to

$$\langle \nabla H(z^1) - \nabla H(z^2) - \gamma(z^1 - z^2) + \xi^1 - \xi^2, u^2 - u^1 \rangle \geq \gamma \|u^1 - u^2\|^2.$$

187 We analyze the three terms on the left hand one by one. Since H is twice continuously
 188 differentiable and $\|\nabla^2 H(z)\| \leq \gamma$ over compact Ω , we have

$$189 \quad (2.2) \quad \begin{aligned} \langle \nabla H(z^1) - \nabla H(z^2), u^2 - u^1 \rangle &\leq \|\nabla H(z^1) - \nabla H(z^2)\| \|u^1 - u^2\| \\ &\leq \gamma \|z^1 - z^2\| \|u^1 - u^2\|. \end{aligned}$$

190 In addition, we also have

$$191 \quad (2.3) \quad \langle -\gamma(z^1 - z^2), u^2 - u^1 \rangle \leq \gamma \|z^1 - z^2\| \|u^1 - u^2\|.$$

192 Now we turn to the third term. Let $w^i = ((W_1^i)^\top, \dots, (W_1^i)^\top, \dots, (W_L^i)^\top, \dots, (W_L^i)^\top)^\top$ and
 193 $\lambda^i = (((\alpha^1)^i)^\top, \dots, ((\alpha^L)^i)^\top)^\top$, $i = 1, 2$. It is not difficult to see that

$$194 \quad \begin{aligned} \langle \xi^1 - \xi^2, u^2 - u^1 \rangle &= \langle \zeta^1 - \zeta^2, w^2 - w^1 \rangle \\ &= \sum_{\ell=1}^L \sum_{j=1}^{n_{\ell-1}} \langle (\alpha_j^\ell)^1 \zeta_{\ell,j}^1 - (\alpha_j^\ell)^2 \zeta_{\ell,j}^2, (W_\ell^2)_{\cdot j} - (W_\ell^1)_{\cdot j} \rangle, \end{aligned}$$

195 where $\zeta_{\ell,j}^i \in \partial \|\cdot\|((W_\ell^i)_{\cdot j})$, $i = 1, 2$. We can consider each item of the third term
 196 separately. For $1 \leq j \leq n_{\ell-1}$, we have

$$197 \quad (2.4) \quad \begin{aligned} &\langle (\alpha_j^\ell)^1 \zeta_{\ell,j}^1 - (\alpha_j^\ell)^2 \zeta_{\ell,j}^2, (W_\ell^2)_{\cdot j} - (W_\ell^1)_{\cdot j} \rangle \\ &= \langle (\alpha_j^\ell)^1 \zeta_{\ell,j}^1 - (\alpha_j^\ell)^1 \zeta_{\ell,j}^2 + (\alpha_j^\ell)^1 \zeta_{\ell,j}^2 - (\alpha_j^\ell)^2 \zeta_{\ell,j}^2, (W_\ell^2)_{\cdot j} - (W_\ell^1)_{\cdot j} \rangle \\ &= (\alpha_j^\ell)^1 \langle \zeta_{\ell,j}^1 - \zeta_{\ell,j}^2, (W_\ell^2)_{\cdot j} - (W_\ell^1)_{\cdot j} \rangle + \langle ((\alpha_j^\ell)^1 - (\alpha_j^\ell)^2) \zeta_{\ell,j}^2, (W_\ell^2)_{\cdot j} - (W_\ell^1)_{\cdot j} \rangle \\ &\leq |(\alpha_j^\ell)^1 - (\alpha_j^\ell)^2| \|\zeta_{\ell,j}^2\| \|(W_\ell^2)_{\cdot j} - (W_\ell^1)_{\cdot j}\| \\ &\leq |(\alpha_j^\ell)^1 - (\alpha_j^\ell)^2| \|u^1 - u^2\|, \end{aligned}$$

198 where the first inequality is from the convexity of the Euclidean norm and the second
 199 inequality is from the fact that $\|\zeta_{\ell,j}^2\| \leq 1$. Combining (2.2), (2.3) and (2.4), we have

$$200 \quad (2.5) \quad \begin{aligned} \|u^1 - u^2\| &\leq 2\|z^1 - z^2\| + \frac{1}{\gamma} \sum_{\ell=1}^L \sum_{j=1}^{n_{\ell-1}} |(\alpha_j^\ell)^1 - (\alpha_j^\ell)^2| \\ &\leq \kappa (\|z^1 - z^2\| + \|\lambda^1 - \lambda^2\|), \end{aligned}$$

201 where $\kappa := \max\{2, \frac{\sqrt{r}}{\gamma}\}$. Hence (2.1) holds. \square

202 **3. Smooth approximation of problem (1.3).** The nonsmoothness of (1.3)
 203 comes from the group sparse regularization term Q in the objective function of its
 204 lower level problem (1.4). In this paper, we use the smoothing function Q_μ in (1.6)
 205 and G_μ in (1.5) as smoothing functions of Q and G , respectively, where $\mu > 0$ is the
 206 smoothing parameter. Properties of the continuity and differentiability of smoothing
 207 function Q_μ can be directly derived from some existing literature (see for example
 208 [36]), and readily extended to G_μ .

209 We consider the following smooth approximation of problem (1.3):

$$210 \quad (3.1) \quad \min_{\lambda, z, u} F(u) \quad \text{s.t.} \quad \lambda \geq 0, \quad z \in \Omega, \quad u = u_\mu(\lambda, z),$$

211 where $u_\mu(\lambda, z)$ is the unique solution of the following lower level problem:

$$212 \quad (3.2) \quad \min_u G_\mu(u; \lambda, z) \quad \text{s.t.} \quad u \in \Omega.$$

Obviously, $u(\lambda, z) = u_\mu(\lambda, z)$ when $\mu = 0$. Since for any fixed $\mu \geq 0$, $\lambda \geq 0$ and $z \in \Omega$, $G_\mu(\cdot; \lambda, z)$ is a strongly convex function and Ω is a convex compact set, $u_\mu(\cdot, \cdot)$ is the unique solution of (3.2). In the following, we investigate properties of the solution function $u_\mu(\cdot, \cdot)$ of problem (3.2) for $\mu > 0$.

PROPOSITION 3.1. *For any $\mu > 0$, the solution function $u_\mu : \mathbb{R}_+^r \times \Omega \rightarrow \mathbb{R}^q$ is Lipschitz continuous with Lipschitz constant $\kappa := \max\{2, \frac{\sqrt{r}}{\gamma}\}$, which is independent of μ , i.e., for any $(\lambda^1, z^1), (\lambda^2, z^2) \in \mathbb{R}_+^r \times \Omega$,*

$$(3.3) \quad \|u_\mu(\lambda^1, z^1) - u_\mu(\lambda^2, z^2)\| \leq \kappa(\|z^1 - z^2\| + \|\lambda^1 - \lambda^2\|).$$

Proof. The proof can be directly derived following the proof of Proposition 2.5 with

$$\zeta_{\ell,j}^i = \frac{(W_\ell^i)_{\cdot,j}}{\sqrt{\|(W_\ell^i)_{\cdot,j}\|^2 + \mu}},$$

and $\|\zeta_{\ell,j}^i\| \leq 1$. □

PROPOSITION 3.2. *For any $(\tilde{\lambda}, \tilde{z}, \tilde{\mu}) \in \mathbb{R}_+^r \times \Omega \times [0, 1]$, we have*

$$(3.4) \quad \lim_{(\lambda, z, \mu) \rightarrow (\tilde{\lambda}, \tilde{z}, \tilde{\mu})} u_\mu(\lambda, z) = u_{\tilde{\mu}}(\tilde{\lambda}, \tilde{z}).$$

Proof. Since $G_\mu(u; \lambda, z)$ is continuous with respect to (λ, z, μ) and Ω is a compact set, we know that for the lower level problem (3.2), the solution set mapping denoted by $\hat{S} : \mathbb{R}_+^r \times \Omega \times [0, 1] \rightrightarrows \Omega$ with $\hat{S}(\lambda, z, \mu) = \{u_\mu(\lambda, z)\}$ is upper semicontinuous with respect to (λ, z, μ) according to [5, Proposition 4.4]. Since for any $\lambda \in \mathbb{R}_+^r$, $z \in \Omega$, $\mu \in [0, 1]$, $\hat{S}(\lambda, z, \mu)$ is singleton, by the definition of upper semicontinuous multifunction [5, Section 4.1], we obtain the continuity of $u_\mu(\lambda, z)$. □

The following proposition is based on Proposition 3.2, and will be used in the proof of Theorem 3.4.

PROPOSITION 3.3. *If $(\lambda_\mu, z_\mu, u_\mu)$ is a feasible point of (3.1), then any accumulation point of $(\lambda_\mu, z_\mu, u_\mu)$ when $\mu \downarrow 0$ is a feasible point of (1.3).*

THEOREM 3.4. *If $(\lambda_\mu, z_\mu, u_\mu)$ is a global optimal solution of problem (3.1), then any accumulation point of $(\lambda_\mu, z_\mu, u_\mu)$ when $\mu \downarrow 0$ is a global optimal solution of problem (1.3).*

Proof. Let (λ^*, z^*, u^*) be an accumulation point of $(\lambda_\mu, z_\mu, u_\mu)$ when $\mu \downarrow 0$. According to Proposition 3.3, (λ^*, z^*, u^*) is a feasible point of (1.3). Assume that there exists a feasible point $(\tilde{\lambda}, \tilde{z}, \tilde{u})$ of problem (1.3) such that $F(\tilde{u}) < F(u^*)$. Due to the continuity of F , there exist δ_1, δ_2 such that for all $u^1 \in B(\tilde{u}, \delta_1)$ and $u^2 \in B(u^*, \delta_2)$, we have $F(u^1) < F(u^2)$. Notice that the solution $u_\mu(\tilde{\lambda}, \tilde{z})$ of lower level problem (3.2) converges to \tilde{u} when $\mu \downarrow 0$, where $(\tilde{\lambda}, \tilde{z})$ is fixed. Letting $\tilde{\mu}$ be sufficiently small such that $\tilde{u}_{\tilde{\mu}} := u_{\tilde{\mu}}(\tilde{\lambda}, \tilde{z}) \in B(\tilde{u}, \delta_1)$ and $u_{\tilde{\mu}} \in B(u^*, \delta_2)$, we have $F(\tilde{u}_{\tilde{\mu}}) < F(u_{\tilde{\mu}})$, which obviously contradicts the global optimality of $(\lambda_{\tilde{\mu}}, z_{\tilde{\mu}}, u_{\tilde{\mu}})$. □

4. Smoothing implicit function method for problem (3.1). According to Theorems 2.2 and 2.3, the global (or local) optimal solutions of problem (1.3) correspond to the global (or local) optimal solutions of (1.1) under some assumptions. Further, due to Theorem 3.4, any accumulation point of global optimal solutions of problem (3.1) is the global optimal solution of problem (1.3) as the smoothing parameter μ goes to zero. Thus we focus on solving problem (3.1) with sufficiently small μ hereafter. For the ease of statement, we let $y = (\lambda^\top, z^\top)^\top$ and omit subscript μ .

Obviously, problem (3.1) can be equivalently transformed to

$$(4.1) \quad \min_{y,u} F(u) \quad \text{s.t. } y \in \mathbb{R}_+^r \times \Omega, \Phi(y, u) = 0,$$

where $\Phi(y, u) := u - \Pi_\Omega(u - \tau(\nabla H(z) + \gamma(u - z) + \nabla_u Q_\mu(w; \lambda)))$ with fixed $\tau > 0$, and $\Pi_\Omega : \mathbb{R}^q \rightarrow \Omega$ is the projection operator.

By substituting unique solution $u(y)$ (subscript μ is omitted for brevity) into objective function F , problem (3.1) can be equivalently transformed to

$$(4.2) \quad \min_y \tilde{F}(y) \quad \text{s.t. } y \in \mathbb{R}_+^r \times \Omega,$$

where $\tilde{F}(y) := F(u(y))$.

4.1. Smoothing approximation of problem (4.1). Since operator Π_Ω is not differentiable, we use the smoothing function proposed in [4] to approximate Φ , and consider

$$(4.3) \quad \min_{y,u} F(u) \quad \text{s.t. } y \in \mathbb{R}_+^r \times \Omega, \Phi_\nu(y, u) = 0,$$

where Φ_ν is a smoothing function of Φ with smoothing parameter $\nu > 0$. The detailed formulation of Φ_ν can be found in Appendix.

According to Lemma 7.3(iii) and implicit function theorem, there exists a unique solution denoted by $u_\nu(y)$ to $\Phi_\nu(y, u) = 0$ for any fixed $y \in \mathbb{R}_+^r \times \Omega$. Thus problem (4.3) can be equivalently transformed to

$$(4.4) \quad \min_y \tilde{F}_\nu(y) \quad \text{s.t. } y \in \mathbb{R}_+^r \times \Omega,$$

where $\tilde{F}_\nu(y) := F(u_\nu(y))$.

Function Φ_ν based on the smoothing function in [4] enjoys impressive properties, which are presented as follows. Accordingly, $\Phi(y, u) = 0$ and $\Phi_\nu(y, u) = 0$ can have the same solution for a positive smoothing parameter ν .

PROPOSITION 4.1. *For any fixed $y \in \mathbb{R}_+^r \times \Omega$, we have*

$$(4.5) \quad \|\Phi(y, u_\nu(y)) - \Phi_\nu(y, u_\nu(y))\| \leq \frac{\sqrt{q}}{2}\nu,$$

for any $\nu \in (0, 1]$. Moreover, for any fixed $y \in \mathbb{R}_+^r \times \Omega$, there is $\tilde{\nu}$ such that

$$(4.6) \quad u_\nu(y) = u(y) \text{ and } \Phi(y, u_\nu(y)) = \Phi_\nu(y, u_\nu(y)) = 0,$$

for any $\nu \in (0, \tilde{\nu}]$.

Proof. From Lemma 7.3(i), we can obtain (4.5). Then we prove (4.6). Denote $\bar{\phi}(\tilde{y}, \tilde{u}) := \tilde{u} - \tau\phi(\tilde{y}, \tilde{u})$ for any $(\tilde{y}, \tilde{u}) \in \mathbb{R}_+^r \times \Omega \times \Omega$, where ϕ is defined in Appendix. Given any fixed $y \in \mathbb{R}_+^r \times \Omega$, let $I_1 := \{i : \underline{u}_i > \bar{\phi}_i(y, u(y))\}$, $I_2 := \{i : \underline{u}_i \leq \bar{\phi}_i(y, u(y))\}$, $I_3 := \{i : \bar{u}_i < \bar{\phi}_i(y, u(y))\}$, $\rho_1 = \min\{3, \underline{u}_i - \bar{\phi}_i(y, u(y)) : i \in I_1\}$, $\rho_2 = \min\{3, \bar{\phi}_i(y, u(y)) - \bar{u}_i : i \in I_3\}$. Denote

$$(4.7) \quad \tilde{\nu} = \min\{(\rho_1/3)^2, (\rho_2/3)^2\}.$$

In order to prove (4.6), it suffices to show that

$$(4.8) \quad \psi_\nu^i(\bar{\phi}_i(y, u(y))) = \Pi_{[\underline{u}_i, \bar{u}_i]}(\bar{\phi}_i(y, u(y)))$$

holds for $\nu \in (0, \tilde{\nu}]$ and $i = 1, \dots, q$. Actually, it is obvious that (4.8) holds for $i \in I_2$.
 Next, for $i \in I_1$, since $\tilde{\nu} \leq (\rho_1/3)^2 \leq 1$, we have

$$\bar{\phi}_i(y, u(y)) \leq \underline{u}_i - \rho_1 \leq \underline{u}_i - 3\sqrt{\tilde{\nu}} \leq \underline{u}_i - \nu - 2\sqrt{\nu},$$

for $\nu \in (0, \tilde{\nu}]$. According to Lemma 7.1(ii), (4.8) holds for $i \in I_1$. Similarly, we can prove that (4.8) holds for $i \in I_3$. Therefore, (4.8) holds for $\nu \in (0, \tilde{\nu}]$ and $i = 1, \dots, q$. \square

PROPOSITION 4.2. *If (y_ν, u_ν) is a global optimal solution of problem (4.3), then any accumulation point of (y_ν, u_ν) when $\nu \downarrow 0$ is a global optimal solution of problem (4.1).*

Proof. Let (y^*, u^*) be an accumulation point of (y_ν, u_ν) when $\nu \downarrow 0$. For the ease of statement, we do not take the subsequence in the proof. Firstly, we prove that (y^*, u^*) is feasible for problem (4.1). Let $y = y_\nu$ in (4.5). Noting that $\Phi_\nu(y_\nu, u_\nu) = 0$ for $\nu > 0$, we have

$$(4.9) \quad \|\Phi(y_\nu, u_\nu)\| = \|\Phi(y_\nu, u_\nu) - \Phi_\nu(y_\nu, u_\nu)\| \leq \frac{\sqrt{q}}{2}\nu.$$

Letting $\nu \downarrow 0$ in (4.9), we have $\Phi(y^*, u^*) = 0$, which implies that $u^* = u(y^*)$ and (y^*, u^*) is feasible for problem (4.1). Then we show that (y^*, u^*) is a global optimal solution of problem (4.1). We prove this by contradiction. Assume that there exists a feasible point (\tilde{y}, \tilde{u}) of problem (4.1) such that $F(\tilde{u}) < F(u^*)$. Since (y_ν, u_ν) is a global optimal solution of problem (4.3), we have $F(u_\nu(\tilde{y})) \geq F(u_\nu)$. Letting $y = \tilde{y}$ and $\nu \downarrow 0$ in (4.5), we can obtain that $\lim_{\nu \downarrow 0} u_\nu(\tilde{y}) = \tilde{u}$, which implies that $F(\tilde{u}) \geq F(u^*)$.

This contradicts the foregoing assumption. So we have proved the conclusion. \square

If y is a local optimal solution of (4.2), then it satisfies $0 \in \partial \tilde{F}(y) + N_{\mathbb{R}_+^r \times \Omega}(y)$. Via [9, Theorem 2.6.6], the above inclusion can be transformed to

$$(4.10) \quad 0 \in (\partial u(y))^\top \nabla F(u(y)) + N_{\mathbb{R}_+^r \times \Omega}(y).$$

Nevertheless, (4.10) involves the subdifferential of implicit function $u(\cdot)$, which is kind of elusive. So we introduce the concept of a weak Clarke stationary point for problem (4.2). Let $u = u(y)$. We call $y \in \mathbb{R}_+^r \times \Omega$ a weak Clarke stationary point of (4.2) if there exist $V_1 \in \partial_u \Phi(y, u)$ and $V_2 \in \partial_y \Phi(y, u)$ such that (y, u) satisfies that

$$(4.11) \quad 0 \in (-(V_1)^{-1}V_2)^\top \nabla F(u(y)) + N_{\mathbb{R}_+^r \times \Omega}(y).$$

Remark 4.3. Here we give the explicit form of $\partial \Phi(y, u)$ for $(y, u) \in \mathbb{R}_+^r \times \Omega \times \Omega$. Define

$$D(y, u) := \left\{ \text{diag}(a) : a_i \in \begin{cases} \{1\}, & \text{if } u_i - \tau \phi_i(y, u) \in (\underline{u}_i, \bar{u}_i), \\ \{0\}, & \text{if } u_i - \tau \phi_i(y, u) \notin [\underline{u}_i, \bar{u}_i], \\ [0, 1], & \text{otherwise,} \end{cases} \quad i = 1, \dots, q \right\},$$

where ϕ is defined in Appendix. Using the chain rule, we can derive that

$$(4.12) \quad \begin{aligned} \partial_u \Phi(y, u) &= \{(\tau\gamma - 1)D + I_q + \tau D \nabla_u^2 Q_\mu(w; \lambda) : D \in D(y, u)\}, \\ \partial_y \Phi(y, u) &= \{\tau D J_y \nabla_u Q_\mu(w; \lambda) + \tau D(0, \nabla^2 H(z) - \gamma I_q) : D \in D(y, u)\}. \end{aligned}$$

Remark 4.4. Actually, $S_\Phi := \{-(V_1)^{-1}V_2 : V_1 \in \partial_u \Phi(y, u), V_2 \in \partial_y \Phi(y, u)\}$ is an approximation of $\partial u(y)$ in (4.10). For example, when Φ is continuously differentiable near (y, u) , we can show that $S_\Phi = \partial u(y)$. In fact, using [9, Proposition 2.2.4], we know that in this case, $\partial \Phi(y, u) = \{J\Phi(y, u)\}$, which indicates

that $V_1 = J_u \Phi(y, u)$ and $V_2 = J_y \Phi(y, u)$. Further, via the implicit function theorem, we know $u(\cdot)$ is continuously differentiable near y and $\partial u(y) = \{Ju(y)\}$, where $Ju(y) = -(J_u \Phi(y, u))^{-1} J_y \Phi(y, u) = -(V_1)^{-1} V_2$.

On the other hand, $y \in \mathbb{R}_+^r \times \Omega$ is said to be a stationary point of problem (4.4) if it satisfies

$$(4.13) \quad 0 \in \nabla \tilde{F}_\nu(y) + N_{\mathbb{R}_+^r \times \Omega}(y).$$

Then we have the following proposition.

PROPOSITION 4.5. *If y_ν is a stationary point of problem (4.4), then any accumulation point of y_ν when $\nu \downarrow 0$ is a weak Clarke stationary point of problem (4.2).*

Proof. Using the implicit function theorem, we have

$$(4.14) \quad \nabla \tilde{F}_\nu(y) = -(J_y \Phi_\nu(y, u_\nu(y)))^\top (J_u \Phi_\nu(y, u_\nu(y)))^{-\top} \nabla F(u_\nu(y)).$$

Combining (4.14) with Lemma 7.3(ii), we can obtain the conclusion. \square

4.2. Smoothing implicit function method. Motivated by Propositions 4.1, 4.2, and 4.5, problem (4.4) is a satisfying approximation of problem (4.2) for ν sufficiently small. In what follows, we will design a smoothing method where ν will eventually be small enough. The framework of the smoothing implicit function method is exhibited in Algorithm 4.1.

Algorithm 4.1 Smoothing implicit function method

Require: Choose parameters $\nu^0 \in (0, 1]$, $\bar{\nu} \in (0, \nu^0]$, $\delta_1 > 0$, $\delta_2 \in (0, 1)$, initial point $y^0 \in \mathbb{R}_+^r \times \Omega$, stepsize $\theta > 0$, tolerances $\bar{\epsilon}, \epsilon_k \in (0, 1)$ for $k = 0, 1, 2, \dots$, and maximum number of iterations k_{\max} .

- 1: **for** $k = 0, 1, 2, \dots$ **do**
- 2: Find u^k such that $\|\Phi_{\nu^k}(y^k, u^k)\| \leq \epsilon_k$.
- 3: Find q^k such that $\|(J_u \Phi_{\nu^k}(y^k, u^k))^\top q^k - \nabla F(u^k)\| \leq \epsilon_k$.
- 4: Compute $p^k = -(J_y \Phi_{\nu^k}(y^k, u^k))^\top q^k$.
- 5: Let

$$y^{k+1} = \Pi_{\mathbb{R}_+^r \times \Omega}(y^k - \theta p^k).$$

- 6: If $\|y^k - \Pi_{\mathbb{R}_+^r \times \Omega}(y^k - \theta p^k)\| \geq \delta_1 \nu^k$, set $\nu^{k+1} = \nu^k$; otherwise, choose $\nu^{k+1} = \max\{\bar{\nu}, \delta_2 \nu^k\}$.
 - 7: If $\|y^{k+1} - y^k\| \leq \bar{\epsilon}$ or $k = k_{\max}$, terminate, and return y^k and u^k .
 - 8: **end for**
-

Note that $\{\nu^k\}$ in Algorithm 4.1 is lower bounded by $\bar{\nu}$ due to step 6, which guarantees that stepsize θ satisfying the assumptions for the convergence of Algorithm 4.1 can be found (see Proposition 4.7 and Lemma 4.9). There exists a trade-off in choosing $\bar{\nu}$. Actually, due to Propositions 4.2 and 4.5, $\bar{\nu}$ should approach 0 in terms of smoothing approximations, which, however, will lead to very small stepsize θ . In numerical experiments, $\bar{\nu}$ is tuned empirically from a set of given parameters.

The following assumption is about the boundedness of $\{\lambda^k\}$.

ASSUMPTION 4.6. *Let $\{y^k\}$ be the sequence generated by Algorithm 4.1. Assume that $\{\lambda^k\}$ is contained in a convex compact set U .*

Now we give some notations. Since F is twice continuously differentiable over Ω , F and ∇F are Lipschitz continuous over Ω with Lipschitz constants ℓ_F and L_F

respectively. Similarly, ∇Q_μ is Lipschitz continuous over $U \times \Omega$ with Lipschitz constant denoted by L_Q . Note that u_k in step 2 of Algorithm 4.1 may not be in Ω . Nevertheless, due to Lemma 7.3(vi) and the boundedness of $\{\epsilon_k\}$, there exists constant $C > 0$ such that $\{u_k\} \subset \bar{\Omega} := [\underline{u} - Ce_q, \bar{u} + Ce_q]$. Since the analysis involving Ω can be extended to $\bar{\Omega}$, we will assume that $u_k \in \Omega$ in this paper for simplicity.

Using Lemma 7.3, we can prove the following proposition.

PROPOSITION 4.7. *For $\nu \in [\bar{\nu}, 1]$, there exists $\tilde{L} > 0$ not related to ν such that*

$$(4.15) \quad \|\nabla \tilde{F}_\nu(y^1) - \nabla \tilde{F}_\nu(y^2)\| \leq \tilde{L} \|y^1 - y^2\|$$

for any $y^1, y^2 \in U \times \Omega$.

Proof. The Lipschitz continuity of $\nabla \tilde{F}_\nu$ is clear from (4.14) and Lemma 7.3(iv)(v). Since ν is lower bounded by $\bar{\nu} > 0$, \tilde{L} is not related to ν by Lemma 7.3(iv). \square

The following lemma shows that p^k approximates $\nabla \tilde{F}_{\nu^k}(y^k)$ well.

LEMMA 4.8. *Let Assumption 4.6 hold. Assume that $\tau\gamma < 1$, $\gamma > L_Q$, and $\sum_{k=0}^{\infty} \epsilon^k < \infty$ in Algorithm 4.1. Then there exists $\bar{k}_1 > 0$ and $\tilde{M} > 0$ such that*

$$(4.16) \quad \|\nabla \tilde{F}_{\nu^k}(y^k) - p^k\| \leq \tilde{M} \epsilon_k,$$

for $k \geq \bar{k}_1$.

Proof. From Algorithm 4.1, we know that $\bar{\nu} \leq \nu^k \leq \nu^0$ for $k \geq 0$. Let

$$\begin{aligned} J_u^k &:= J_u \Phi_{\nu^k}(y^k, u_{\nu^k}(y^k)), \quad \tilde{J}_u^k := J_u \Phi_{\nu^k}(y^k, u^k), \\ J_y^k &:= J_y \Phi_{\nu^k}(y^k, u_{\nu^k}(y^k)), \quad \tilde{J}_y^k := J_y \Phi_{\nu^k}(y^k, u^k), \\ f^k &:= \nabla F(u_{\nu^k}(y^k)), \quad \tilde{f}^k := \nabla F(u^k). \end{aligned}$$

Due to Lemma 7.3(iv), there exists upper bound $M_1 > 0$ for the norms of the above terms. Since $\bar{\nu} \leq \nu^k \leq \nu^0$ for $k \geq 0$, from Lemma 7.3(iv)(v), there exists upper bound $M_2 > 0$ for $\{\|(J_u^k)^{-1}\|\}, \{\|(\tilde{J}_u^k)^{-1}\|\}, \{\|\ell_{\nu^k}^u\|\}$ and $\{\|\ell_{\nu^k}^y\|\}$ as well.

Using Lemma 7.3(vi), we know that $\|u_{\nu^k}(y^k) - u^k\| \leq \frac{\epsilon_k}{\tau(\gamma - L_Q)}$. Let v^k be the solution to $(J_u^k)^\top v^k = f^k$ and \tilde{v}^k be the solution to $(\tilde{J}_u^k)^\top \tilde{v}^k = \tilde{f}^k$. Obviously, $\max\{\|v^k\|, \|\tilde{v}^k\|\} \leq M_1 M_2$ for $k \geq 0$. Now we investigate $\|v^k - \tilde{v}^k\|$. Due to Lemma 7.3(v), we have

$$\|J_u^k - \tilde{J}_u^k\| \leq \frac{\ell_{\nu^k}^u \epsilon_k}{\tau(\gamma - L_Q)}, \quad \|f^k - \tilde{f}^k\| \leq \frac{L_F \epsilon_k}{\tau(\gamma - L_Q)}.$$

Since $\sum_{k=0}^{\infty} \epsilon^k < \infty$, there exists constants $\bar{k}_1, \bar{c}_1 > 0$ such that $\frac{\ell_{\nu^k}^u \epsilon_k \|(J_u^k)^{-\top}\|}{\tau(\gamma - L_Q)} \leq \bar{c}_1 < 1$, for $k \geq \bar{k}_1$. Due to [19, Theorem 7.2], for $k \geq \bar{k}_1$, we have

$$\begin{aligned} \|v^k - \tilde{v}^k\| &\leq \frac{\frac{\epsilon_k}{\tau(\gamma - L_Q)}}{1 - \frac{\ell_{\nu^k}^u \epsilon_k \|(J_u^k)^{-\top}\|}{\tau(\gamma - L_Q)}} (L_F \|(J_u^k)^{-\top}\| + \ell_{\nu^k}^u \|v^k\| \|(J_u^k)^{-\top}\|) \\ &\leq \frac{\epsilon_k}{\tau(\gamma - L_Q)(1 - \bar{c}_1)} (L_F \|(J_u^k)^{-\top}\| + \ell_{\nu^k}^u \|v^k\| \|(J_u^k)^{-\top}\|) \\ &\leq M_3 \epsilon_k, \end{aligned}$$

where $M_3 := \frac{L_F M_2 + M_1 (M_2)^3}{\tau(\gamma - L_Q)(1 - \bar{c}_1)}$.

Then we investigate $\|q^k - v^k\|$. Actually, for $k \geq \bar{k}_1$,

$$\begin{aligned}\|q^k - v^k\| &= \|q^k - \tilde{v}^k + \tilde{v}^k - v^k\| \\ &\leq \|q^k - \tilde{v}^k\| + \|v^k - \tilde{v}^k\| \\ &\leq \|(\tilde{J}_u^k)^{-\top} (\tilde{J}_u^k)^\top (q^k - \tilde{v}^k)\| + \|v^k - \tilde{v}^k\| \\ &\leq \|(\tilde{J}_u^k)^{-\top}\| \|(\tilde{J}_u^k)^\top q^k - \tilde{f}^k\| + \|v^k - \tilde{v}^k\| \\ &\leq (M_2 + M_3)\epsilon_k,\end{aligned}$$

where the last equality follows from the fact that $\|(\tilde{J}_u^k)^\top q^k - \tilde{f}^k\| \leq \epsilon_k$.

Finally, for $k \geq \bar{k}_1$, we have

$$\begin{aligned}\|\nabla \tilde{F}_{\nu^k}(y^k) - p^k\| &= \|(J_y^k)^\top v^k - ((\tilde{J}_y^k)^\top q^k)\| \\ &= \|(J_y^k)^\top v^k - (\tilde{J}_y^k)^\top v^k + (\tilde{J}_y^k)^\top v^k - (\tilde{J}_y^k)^\top q^k\| \\ &\leq \|(J_y^k)^\top v^k - (\tilde{J}_y^k)^\top v^k\| + \|(\tilde{J}_y^k)^\top v^k - (\tilde{J}_y^k)^\top q^k\| \\ &\leq \|J_y^k - \tilde{J}_y^k\| \|v^k\| + \|\tilde{J}_y^k\| \|v^k - q^k\| \\ &\leq \frac{\ell_{\nu^k}^y \epsilon_k \|v^k\|}{\tau(\gamma - L_Q)} + \|\tilde{J}_y^k\| \|v^k - q^k\| \\ &\leq \tilde{M} \epsilon_k,\end{aligned}$$

where the last but one inequality follows from Lemma 7.3(iv), and the final estimate uses $\tilde{M} := \frac{M_1(M_2)^2}{\tau(\gamma - L_Q)} + M_1M_2 + M_1M_3$. \square

LEMMA 4.9. Let assumptions of Lemma 4.8 hold. Assume that $\theta \leq \frac{1}{L}$ in Algorithm 4.1, where \tilde{L} is defined in Proposition 4.7. Then there exists $\bar{k}_2 > 0$ such that $\nu^k = \bar{\nu}$, for $k \geq \bar{k}_2$.

Proof. Denote set $K := \{k : \nu^{k+1} = \max\{\bar{\nu}, \delta_2 \nu^k\}\}$. It suffices to prove that set K is infinite. We prove this by contradiction. Suppose that K is finite. Then there exist $\hat{\nu} > \bar{\nu}$ and $k_0 > 0$ such that for $k \geq k_0$,

$$(4.17) \quad \nu^k = \hat{\nu} \text{ and } \|y^{k+1} - y^k\| \geq \delta_1 \hat{\nu}.$$

From (4.15), we know that $\tilde{F}_{\hat{\nu}}$ satisfies that

$$(4.18) \quad \tilde{F}_{\hat{\nu}}(y_a) \leq \tilde{F}_{\hat{\nu}}(y_b) + \nabla \tilde{F}_{\hat{\nu}}(y_b)^\top (y_a - y_b) + \frac{\tilde{L}}{2} \|y_a - y_b\|^2$$

for any $y_a, y_b \in U \times \Omega$. Due to Lemma 7.2(ii), we have

$$\|\Pi_{\mathbb{R}_+^r \times \Omega}(y_a) - \Pi_{\mathbb{R}_+^r \times \Omega}(y_b)\|^2 \leq (y_a - y_b)^\top (\Pi_{\mathbb{R}_+^r \times \Omega}(y_a) - \Pi_{\mathbb{R}_+^r \times \Omega}(y_b)).$$

Letting $y_a = y^k - \theta p^k$ and $y_b = y^k$ in the above inequality, we can obtain that

$$(4.19) \quad \|y^{k+1} - y^k\|^2 \leq -\theta (p^k)^\top (y^{k+1} - y^k).$$

Let $\bar{k}_2 = \max\{k_0, \bar{k}_1\}$ with \bar{k}_1 defined in Lemma 4.8. Substituting y^{k+1}, y^k into (4.18),

402 for $k \geq \bar{k}_2$, we have

$$\begin{aligned}
& \tilde{F}_{\bar{\nu}}(y^{k+1}) \\
& \leq \tilde{F}_{\bar{\nu}}(y^k) + \nabla \tilde{F}_{\bar{\nu}}(y^k)^\top (y^{k+1} - y^k) + \frac{\tilde{L}}{2} \|y^{k+1} - y^k\|^2 \\
& = \tilde{F}_{\bar{\nu}}(y^k) + (\nabla \tilde{F}_{\bar{\nu}}(y^k) - p^k)^\top (y^{k+1} - y^k) + (p^k)^\top (y^{k+1} - y^k) + \frac{\tilde{L}}{2} \|y^{k+1} - y^k\|^2 \\
& \leq \tilde{F}_{\bar{\nu}}(y^k) + (\nabla \tilde{F}_{\bar{\nu}}(y^k) - p^k)^\top (y^{k+1} - y^k) - \frac{1}{\theta} \|y^{k+1} - y^k\|^2 + \frac{\tilde{L}}{2} \|y^{k+1} - y^k\|^2 \\
& \leq \tilde{F}_{\bar{\nu}}(y^k) + \|\nabla \tilde{F}_{\bar{\nu}}(y^k) - p^k\| \|y^{k+1} - y^k\| - \frac{\tilde{L}}{2} \|y^{k+1} - y^k\|^2 \\
& \leq \tilde{F}_{\bar{\nu}}(y^k) + M\epsilon^k - \frac{\tilde{L}}{2} \|y^{k+1} - y^k\|^2,
\end{aligned}$$

404 where the second inequality holds from (4.19), the third inequality holds from the fact
405 that $\theta \leq \frac{1}{\tilde{L}}$, the last inequality follows from Lemma 4.8 and the boundedness of $\{y^k\}$,
406 and constant $M > 0$ is constructed based on \tilde{M} . So we obtain that

$$407 \quad (4.20) \quad \|y^{k+1} - y^k\|^2 \leq \frac{2}{\tilde{L}} (\tilde{F}_{\bar{\nu}}(y^k) - \tilde{F}_{\bar{\nu}}(y^{k+1}) + M\epsilon^k),$$

408 for $k \geq \bar{k}_2$. Summing (4.20) for $k = \bar{k}_2, \bar{k}_2 + 1, \dots$, we have

$$409 \quad \sum_{k=\bar{k}_2}^{\infty} \|y^{k+1} - y^k\|^2 \leq \frac{2}{\tilde{L}} \left(\tilde{F}_{\bar{\nu}}(y^{\bar{k}_2}) + M \sum_{k=\bar{k}_2}^{\infty} \epsilon^k \right).$$

410 Since $\sum_{k=0}^{\infty} \epsilon^k < \infty$, we know that $\lim_{k \rightarrow \infty} \|y^{k+1} - y^k\| = 0$, which contradicts (4.17). So
411 we have proved the conclusion. \square

412 **THEOREM 4.10.** *Let assumptions of Lemma 4.9 hold. Let (\tilde{y}, \tilde{u}) be an accumula-*
413 *tion point of sequence $\{(y^k, u^k)\}$ generated by Algorithm 4.1. Then \tilde{y} satisfies that*

$$414 \quad (4.21) \quad 0 \in \nabla \tilde{F}_{\bar{\nu}}(\tilde{y}) + N_{\mathbb{R}_+^r \times \Omega}(\tilde{y}),$$

415 where $\nabla \tilde{F}_{\bar{\nu}}(\tilde{y}) = -(J_u \Phi_{\bar{\nu}}(\tilde{y}, \tilde{u}))^{-1} J_y \Phi_{\bar{\nu}}(\tilde{y}, \tilde{u})^\top \nabla F(u_{\bar{\nu}}(\tilde{y}))$.

416 *Proof.* According to the proof of Lemma 4.9, we have

$$417 \quad (4.22) \quad \lim_{k \rightarrow \infty} \|y^k - \Pi_{\mathbb{R}_+^r \times \Omega}(y^k - \theta p^k)\| = 0.$$

418 Via Lemmas 4.8 and 4.9, we have

$$419 \quad (4.23) \quad \|\nabla \tilde{F}_{\bar{\nu}}(y^k) - p^k\| \leq \tilde{M}\epsilon_k,$$

for $k \geq \bar{k}_2$ with \bar{k}_2 defined in Lemma 4.9. By virtue of (4.23), (4.22) can be transformed to

$$\|\tilde{y} - \Pi_{\mathbb{R}_+^r \times \Omega}(\tilde{y} - \theta \nabla \tilde{F}_{\bar{\nu}}(\tilde{y}))\| = 0,$$

420 which is equivalent to (4.21). The explicit form of $\nabla \tilde{F}_{\bar{\nu}}(\tilde{y})$ follows from (4.14). To
421 show that $\tilde{u} = u_{\bar{\nu}}(\tilde{y})$, we utilize Lemma 7.3(vi) and obtain

$$422 \quad (4.24) \quad \|u^k - u_{\bar{\nu}}(y^k)\| \leq \frac{\epsilon_k}{\tau(\gamma - L_Q)},$$

423 for $k \geq \bar{k}_2$. Letting $k \rightarrow \infty$ in both sides of (4.24), we have $\tilde{u} = u_{\bar{\nu}}(\tilde{y})$. \square

5. Numerical experiments. In this section, we will conduct numerical experiments on the feed-forward neural network. The synthetic data and real-life datasets from UCI machine learning repository [26] will be tested respectively.

Algorithm 4.1 will be compared with the Grid Search method, the Random Search method and the Bayesian optimization method, where Random Search method (see [18, 30]) and Bayesian optimization method (see [3, 39]) are also widely used for hyperparameter optimization in machine learning. The Grid Search method is to solve (1.2) for every grid point respectively and determine the best hyperparameter according to the validation error [34]. The Random Search method is basically the same strategy, except that the grid points are chosen randomly. To use Grid Search method and Random Search method, we denote $\alpha_j^\ell = a_0$ for $\ell = 1, 2$ and $j = 1, \dots, n_{\ell-1}$, and choose a_0 from some given set (see [34]). The Bayesian optimization method used in this paper is from [3]. In Grid Search method, Random Search method and Bayesian optimization method, problem (1.2) with fixed λ is solved via ADADELTA [44].

5.1. Tests on synthetic data. The synthetic data are randomly generated in similar way as used in [10, Section 5.1]. We consider bilevel optimization for tuning hyperparameters of 2-layer sparse feed-forward neural networks. We first randomly generate $X^i \sim \mathcal{N}(\zeta, \Sigma_0 \Sigma_0^\top)$ with $\zeta = \text{randn}(n, 1)$ and $\Sigma_0 = \text{randn}(n, 1)$. The activation function σ is the sigmoid function denoted by $\sigma(t) = \frac{1}{1+e^{-t}}$, $t \in \mathbb{R}$. Truth values of W_1^* , W_2^* and $b^{1,*}, b^{2,*}$ are randomly generated as follows. Generate $\bar{W}_1 \in \mathbb{R}^{n_1 \times n}$ and $\bar{W}_2 \in \mathbb{R}^{1 \times n_1}$ from the uniform distribution $\mathcal{U}(-1, 1)$, and choose index sets $J_1 \subseteq \{1, \dots, n\}$ of size $|J_1|$ and $J_2 \subseteq \{1, \dots, n_1\}$ of size $|J_2|$ randomly. Let $(\bar{W}_1)_{\cdot j} = 0$ for $j \in J_1$ and $(\bar{W}_2)_{\cdot j} = 0$ for $j \in J_2$. Denote $W_1^* = \bar{W}_1$ and $W_2^* = \bar{W}_2$, and generate $b^{1,*}, b^{2,*}$ from the uniform distribution $\mathcal{U}(-1, 1)$. Then we generate

$$Y_i = W_2^* \sigma(W_1^* X^i + b^{1,*}) + b^{2,*} + \tilde{Y}_i, \quad i = 1, \dots, \bar{N},$$

where $\tilde{Y}_i \sim 0.05\mathcal{N}(0, 1)$ is the noise. The synthetic data are divided into three groups indexed by integers N_{tr} , N_{va} and N_{te} . Specifically, $\{(X^i, Y^i) : i = 1, \dots, N_{tr}\}$ is the training group, $\{(X^i, Y^i) : i = N_{tr} + 1, \dots, N_{tr} + N_{va}\}$ is the validation group, and $\{(X^i, Y^i) : i = N_{tr} + N_{va} + 1, \dots, \bar{N}\}$ is the test group. We set $\bar{u} = 20 * e_q$ and $\underline{u} = -20 * e_q$.

Denote the calculated solutions by W_1 , W_2 , and b^1, b^2 . The test error is denoted as

$$\text{TestErr} := \frac{1}{N_{te}} \sum_{i=N_{tr}+N_{va}+1}^{\bar{N}} \|W_2 \sigma(W_1 X^i + b^1) + b^2 - Y^i\|^2.$$

The validation error is denoted as

$$\text{ValErr} := \frac{1}{N_{va}} \sum_{i=N_{tr}+1}^{N_{tr}+N_{va}} \|W_2 \sigma(W_1 X^i + b^1) + b^2 - Y^i\|^2.$$

We denote by Z_0 the number of zero columns of W_1 and W_2 . Denote Z_c the number of zero columns that W_1^*, W_2^* and W_1, W_2 have in common. Here the columns of W_1 and W_2 are taken as zero vectors if their Euclidean norms are less than 10^{-3} .

In the experiments, we let $N_{tr} = \lceil 0.6\bar{N} \rceil$ and $N_{va} = \lceil 0.2\bar{N} \rceil$. The remaining data are set to be the test group. We consider nine combinations of $(\bar{N}, n, n_1, |J_1|, |J_2|)$ presented in Table 1.

In the implementation of Algorithm 4.1, we set $\nu^0 = 1$, $\delta_1 = 100$, $\delta_2 = 0.9$, and $\epsilon_k = \frac{0.1}{k^2}$ ($\epsilon_0 = 0.1$). We let $\alpha_j^\ell = 10^{-4}$ for $\ell = 1, 2$ and $j = 1, \dots, n_{\ell-1}$, and take the

Table 1: Datatype

D1	D2	D3
(500,50,10,10,5)	(1000,100,40,30,10)	(2000,200,40,30,10)
D4	D5	D6
(3000,300,50,40,10)	(5000,500,100,80,40)	(5000,1000,100,100,50)
D7	D8	D9
(10000,1000,300,200,100)	(10000,2000,400,300,100)	(10000,3000,500,600,200)

solution of (1.2) calculated via the ADADELTA algorithm as z^0 . The quasi-Newton method in [6] is employed in step 2, and q^k is obtained by the conjugate gradient method. We let $\bar{\epsilon} = 10^{-5}$ and $k_{\max} = 500$.

We set μ and $\bar{\nu}$ among $\{10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}\}$, and employ the setting with the lowest validation error. In order to determine parameter γ , we use the Matlab built-in solver `fmincon` to solve the following problem:

$$(5.1) \quad \max_z \quad \|\nabla^2 H(z)\|_F^2 \quad \text{s.t. } z \in \Omega,$$

where $\|\cdot\|_F$ denotes the Frobenius norm. Denote by $\tilde{\gamma}$ the positive square root of optimal value of problem (5.1). Similarly, we can evaluate L_Q , where we set $U := [10^{-4}, 10^4]^r$. Then we let $\gamma = 2 \max\{\tilde{\gamma}, L_Q\}$, and $\tau = \frac{1}{2\gamma}$. For each setting of μ and $\bar{\nu}$, it is difficult to calculate \tilde{L} in practice, so we can not designate stepsize θ directly. Motivated by [17], we choose stepsize θ from $\{10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1\}$, and accept the one with the lowest validation error.

Some numerical results about datasets $D2$ and $D3$ are exhibited in Fig. 1, where we can find that Algorithm 4.1 performs better when μ and $\bar{\nu}$ are smaller, and the performances are insensitive to the setting of μ and $\bar{\nu}$ when μ and $\bar{\nu}$ are smaller than 10^{-6} . In the implementations, the mini-batch technique [22] is employed to accelerate the computing of Algorithm 4.1, which leads to the oscillations in Fig. 1.

In the Grid Search method, we choose hyperparameter a_0 from set $\{10^{-k} : k = -4, \dots, 4\}$. In the Random Search method, let $a_0 = 10^{-\omega}$, and generate ω 10 times from the uniform distribution $\mathcal{U}(-4, 4)$. For both methods, the hyperparameter with the smallest validation error will be accepted. In the Bayesian optimization method, for $\ell = 1, 2$ and $j = 1, \dots, n_{\ell-1}$, we denote $\alpha_j^\ell = 10^{-\omega_j^\ell}$, and search over the transformed variable ω_j^ℓ , where the search space of ω_j^ℓ is defined as the uniform distribution $\mathcal{U}(-4, 4)$.

For every type of data, 10 examples are randomly generated, and the average results are exhibited in Table 2 and Fig. 2. Here we can see that Algorithm 4.1 performs best in regard to test error and validation error, and the gap widens with the increase of the scale of the data. All methods yield sparse neural networks, and the networks trained via Algorithm 4.1 are sparser when the size is larger. The above numerical experiments are conducted on 2-layer neural networks which can be very wide (see datatypes D8 and D9). However, considering the partially difficult computations in each iteration (solving a nonlinear system via quasi-Newton method and a linear system via conjugate gradient method), Algorithm 4.1 is more suitable for wide but not very deep neural networks.

Denote $\text{StaErr} = \left\| y - \Pi_{\mathbb{R}_+^r \times \Omega}(y - \theta p) \right\|$, where y, p are obtained from the last iteration. The numerical results are presented in Table 3, where ‘‘Iter’’ denotes the

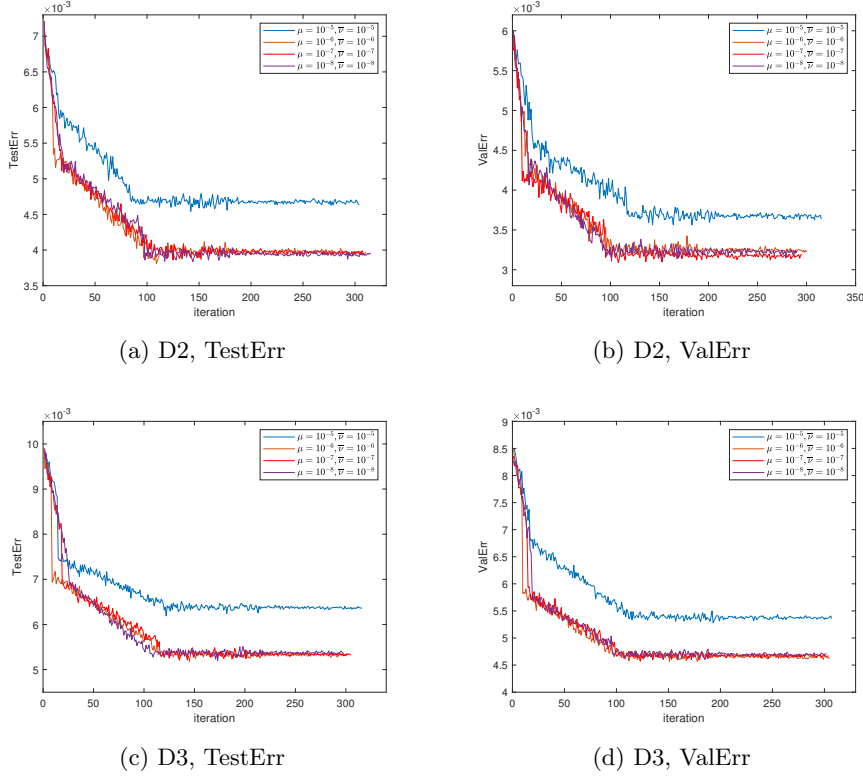


Fig. 1: Comparison of Algorithm 4.1 with varying μ and $\bar{\nu}$

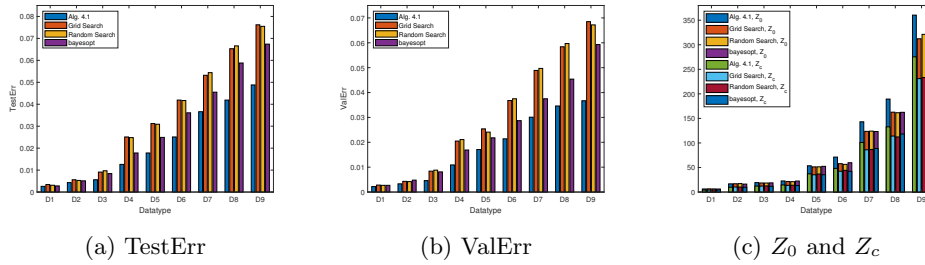


Fig. 2: Numerical results for synthetic data

average number of outer iterations, and “Time” denotes the average CPU time in seconds.

5.2. Tests on real-life data. Now we conduct the experiments on the real-life datasets. These datasets are downloaded from UCI machine learning repository [26], including Higher Education Students Performance Evaluation Dataset (Student), Facebook Comment Volume Dataset (Facebook), Insurance Company Benchmark

Table 2: Numerical results for synthetic data

	Alg	TestErr	ValErr	Z_0	Z_c
D1	Alg. 4.1	0.0026	0.0022	6.3	4.1
	Grid Search	0.0034	0.0028	6.5	4.1
	Random Search	0.0031	0.0027	6.4	4.4
	bayesopt	0.0028	0.0027	6.2	4.4
D2	Alg. 4.1	0.0043	0.0033	16.7	9.9
	Grid Search	0.0056	0.0043	16.9	10.3
	Random Search	0.0053	0.0042	17.2	10.2
	bayesopt	0.0051	0.0048	16.2	9.8
D3	Alg. 4.1	0.0056	0.0046	19.2	12.2
	Grid Search	0.0091	0.0084	18.5	12.2
	Random Search	0.0097	0.0088	18.4	12.5
	bayesopt	0.0084	0.0081	18.7	11.8
D4	Alg. 4.1	0.0126	0.0109	22.6	14.5
	Grid Search	0.0251	0.0205	21.5	13.7
	Random Search	0.0248	0.0211	21.1	13.9
	bayesopt	0.0178	0.0169	22.4	13.2
D5	Alg. 4.1	0.0178	0.0171	53.5	37.1
	Grid Search	0.0312	0.0254	51.3	35.2
	Random Search	0.0309	0.0241	51.4	36.7
	bayesopt	0.0249	0.0218	52.4	35.3
D6	Alg. 4.1	0.0251	0.0214	71.2	48.2
	Grid Search	0.0419	0.0368	57.8	42.4
	Random Search	0.0417	0.0375	56.4	44.2
	bayesopt	0.0361	0.0287	59.7	42.1
D7	Alg. 4.1	0.0366	0.0301	143.1	100.9
	Grid Search	0.0532	0.0489	123.6	86.1
	Random Search	0.0544	0.0497	124.1	86.7
	bayesopt	0.0455	0.0375	123.3	88.7
D8	Alg. 4.1	0.0419	0.0346	189.4	132.8
	Grid Search	0.0653	0.0584	162.7	114.1
	Random Search	0.0666	0.0597	161.6	112.2
	bayesopt	0.0588	0.0454	162.4	118.2
D9	Alg. 4.1	0.0488	0.0367	360.4	275.4
	Grid Search	0.0762	0.0685	312.2	231.1
	Random Search	0.0755	0.0672	321.2	233.2
	bayesopt	0.0674	0.0593	321.7	237.4

Dataset (Insurance) and BlogFeedback Dataset (Blog).

We use the min-max normalization technique to rescale the data to $[0, 1]$. The settings of the algorithms and evaluation criteria are same as those in the last subsection. The numerical results are exhibited in Table 4 and Fig. 3. Here we can find that Algorithm 4.1 performs better than Grid Search method, Random Search method and Bayesian optimization method, especially in terms of Student dataset and Facebook dataset.

Table 3: Numerical results for synthetic data

	D1	D2	D3	D4	D5
StaErr	2.234e-06	4.162e-06	3.462e-06	1.181e-06	4.842e-06
Iter	303.4	305.8	321.6	311.4	348.5
Time	10.1	35.4	60.5	99.7	255.2
	D6	D7	D8	D9	
StaErr	9.467e-06	5.233e-06	8.462e-06	4.238e-06	
Iter	309.1	343.2	356.8	355.5	
Time	469.5	787.1	1449.9	2926.3	

Table 4: Numerical results for real-life data

Dataset	(\tilde{N}, m, n_1, n)	Alg	TestErr	ValErr	Z_0
Student	(145,1,10,31)	Alg. 4.1	0.0603	0.1319	17.9
		Grid Search	0.0739	0.2008	15.4
		Random Search	0.0789	0.2106	15.2
		bayesopt	0.0751	0.1713	15.8
Facebook	(40949,1,10,53)	Alg. 4.1	0.1134	0.1458	4.8
		Grid Search	0.1233	0.2501	3.4
		Random Search	0.1167	0.2447	3.6
		bayesopt	0.1198	0.1514	4.9
Insurance	(5822,1,20,85)	Alg. 4.1	0.2269	0.2163	20.7
		Grid Search	0.2419	0.2383	22.7
		Random Search	0.2329	0.2363	22.5
		bayesopt	0.2355	0.2214	22.3
Blog	(52397,1,50,280)	Alg. 4.1	0.0119	0.0217	33.4
		Grid Search	0.0193	0.0292	33.9
		Random Search	0.0201	0.0298	33.1
		bayesopt	0.0165	0.0265	34.4

6. Conclusion. In the bilevel optimization problem (1.1) for tuning hyperparameters of sparse neural networks, lower level problem (1.2) is nonconvex and non-smooth, which makes the problems computationally intractable. By using the structure of the objective function in (1.2), a convex majorant approach with smooth approximations is proposed in this paper. In particular, we introduce a convex majorant function $G(\cdot; \lambda, z)$ to approximate the objective function of the lower level problem (1.2), and establish the relationship between the original bilevel optimization (1.1) and the bilevel optimization (1.3) with $G(\cdot; \lambda, z)$ regarding global and local minimizers. Then we use smoothing function $G_\mu(\cdot; \lambda, z)$ to approximate $G(\cdot; \lambda, z)$, and derive the convergence of global minimizers to those of problem (1.3) with smoothing parameter μ converging to zero. The approximate bilevel optimization problem (3.1) with $G_\mu(\cdot; \lambda, z)$ is solved via the smoothing implicit function method. The numerical experiments including the tests on the data from machine learning repository indicate that the convex majorant approach performs better than the Grid Search method, the Random Search method and the Bayesian optimization method.

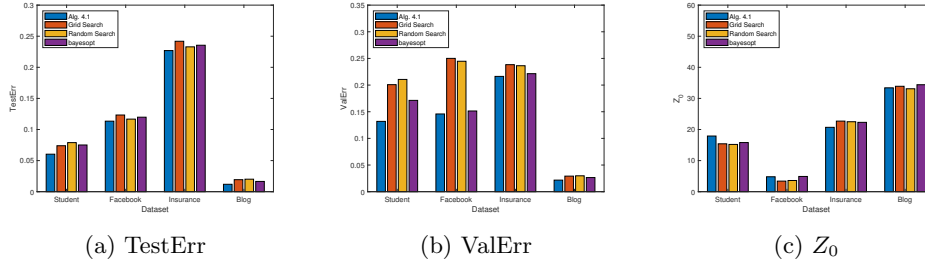


Fig. 3: Numerical results for real-life data

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7. APPENDIX. Note that the nonsmoothness of Φ is due to projection operator Π_Ω . For any $u \in \mathbb{R}^q$, from [4, equation (1.6)], we have

$$\Pi_\Omega(u) = \max\{\underline{u} - u, 0\} + u - \max\{u - \bar{u}, 0\},$$

where “max” has to be understood in componentwise fashion. Hence, the core of the smoothing method is to introduce a surrogate smoothing function of $\max\{\cdot, 0\}$

with some nice properties. In [4, Section 3.2], a smoothing function of $\max\{\cdot, 0\}$ is proposed as follows:

$$(7.1) \quad \varphi_\nu(t) = \begin{cases} 0, & \text{if } t \leq 0, \\ \frac{t^2}{2\nu}, & \text{if } 0 < t \leq \nu, \\ \frac{1}{4}(t - \nu)^2 + t - \frac{1}{2}\nu, & \text{if } \nu < t \leq \nu + \sqrt{\nu}, \\ -\frac{1}{4}(t - \nu - 2\sqrt{\nu})^2 + t, & \text{if } \nu + \sqrt{\nu} < t \leq \nu + 2\sqrt{\nu}, \\ t, & \text{if } t > \nu + 2\sqrt{\nu}, \end{cases}$$

where $\nu > 0$.

Using φ_ν , a smoothing function of the projection operator Π_Ω can be defined as follows:

$$(7.2) \quad \Psi_\nu(u) = (\psi_\nu^1(u_1), \dots, \psi_\nu^2(u_2), \dots, \psi_\nu^q(u_q))^\top,$$

where, for any $t \in \mathbb{R}$,

$$(7.3) \quad \psi_\nu^i(t) = \varphi_\nu(\underline{u}_i - t) + t - \varphi_\nu(t - \bar{u}_i), \quad i = 1, 2, \dots, q.$$

Denote $\phi(y, u) := \nabla H(z) + \gamma(u - z) + \nabla_u Q_\mu(w; \lambda)$. Then the smoothing function of Φ can be defined as

$$(7.4) \quad \Phi_\nu(y, u) = u - \Psi_\nu(u - \tau\phi(y, u)).$$

Then we present some properties of smoothing functions from [4, Proposition 3.4], which are used in this paper.

LEMMA 7.1. *For any fixed $\nu \in (0, 1]$, functions ψ_ν^i in (7.2), $i = 1, 2, \dots, q$, are continuously differentiable and satisfy the following properties:*

- (i) $|\psi_\nu^i(t) - \Pi_{[\underline{u}_i, \bar{u}_i]}(t)| \leq \frac{1}{2}\nu$, for any $t \in \mathbb{R}$.
- (ii) $\psi_\nu^i(t) = \Pi_{[\underline{u}_i, \bar{u}_i]}(t)$ if $t \leq \underline{u}_i - \nu - 2\sqrt{\nu}$ or $\underline{u}_i \leq t \leq \bar{u}_i$ or $t \geq \bar{u}_i + \nu + 2\sqrt{\nu}$.
- (iii) $|(\psi_\nu^i)'(t)| \leq 1$, for any $t \in \mathbb{R}$, where $(\psi_\nu^i)'(t)$ denotes the derivative of ψ_ν^i at t .

- (iv) $|\psi_\nu^i(t^1) - \psi_\nu^i(t^2)| \leq |t^1 - t^2|$, for any $t^1, t^2 \in \mathbb{R}$.

- (v) There exists constant L_ν^i such that, for any $t^1, t^2 \in \mathbb{R}$, $|(\psi_\nu^i)'(t^1) - (\psi_\nu^i)'(t^2)| \leq L_\nu^i |t^1 - t^2|$. Moreover, there exists $M^i > 0$ such that $L_\nu^i \leq \frac{M^i}{\nu}$ for $\nu \in (0, 1]$.

Before introducing the properties of Φ_ν , we give some basic properties of the projection operator, which can be found in [16, Theorem 1.5.5].

LEMMA 7.2. *Let $\Gamma \subset \mathbb{R}^s$ be a nonempty closed convex set. Then we have the following conclusions.*

- (i) For any $x_a, x_b \in \mathbb{R}^s$, $\|\Pi_\Gamma(x_a) - \Pi_\Gamma(x_b)\| \leq \|x_a - x_b\|$.
- (ii) For any $x_a, x_b \in \mathbb{R}^s$, $(\Pi_\Gamma(x_a) - \Pi_\Gamma(x_b))^\top (x_a - x_b) \geq \|\Pi_\Gamma(x_a) - \Pi_\Gamma(x_b)\|^2$.

LEMMA 7.3. *For any $\nu \in (0, 1]$, Φ_ν is continuously differentiable over $\mathbb{R}_+^r \times \Omega \times \Omega$, and satisfies the following properties:*

- (i) $\|\Phi_\nu(\tilde{y}, \tilde{u}) - \Phi(\tilde{y}, \tilde{u})\| \leq \frac{\sqrt{q}}{2}\nu$, for any $(\tilde{y}, \tilde{u}) \in \mathbb{R}_+^r \times \Omega \times \Omega$.
- (ii) $\lim_{(y, u) \rightarrow (\tilde{y}, \tilde{u}), \nu \downarrow 0} \text{dist}(J\Phi_\nu(y, u), \partial\Phi(\tilde{y}, \tilde{u})) = 0$, for any $(\tilde{y}, \tilde{u}) \in \mathbb{R}_+^r \times \Omega \times \Omega$,

where dist denotes the distance.

- (iii) $J_u \Phi_\nu(\tilde{y}, \tilde{u})$ is invertible, for any $(\tilde{y}, \tilde{u}) \in \mathbb{R}_+^r \times \Omega \times \Omega$.

(iv) There exist constants $b^u, b^y, \tilde{b}_\nu^u > 0$ such that for any $(\tilde{y}, \tilde{u}) \in U \times \Omega \times \Omega$,

$$\|J_u \Phi_\nu(\tilde{y}, \tilde{u})\| \leq b^u, \|J_y \Phi_\nu(\tilde{y}, \tilde{u})\| \leq b^y, \|(J_u \Phi_\nu(\tilde{y}, \tilde{u}))^{-1}\| \leq \tilde{b}_\nu^u,$$

where U is a compact set introduced in Assumption 4.6. Moreover, for any $0 < \tilde{c} < 1$, there exists $\tilde{b}^u > 0$ such that $\|(J_u \Phi_\nu(\tilde{y}, \tilde{u}))^{-1}\| \leq \tilde{b}^u$ for $(\tilde{y}, \tilde{u}) \in U \times \Omega \times \Omega$ and $\nu \in [\tilde{c}, 1]$.

(v) $J_u \Phi_\nu(\cdot, \cdot)$, $J_y \Phi_\nu(\cdot, \cdot)$ and $(J_u \Phi_\nu(\cdot, \cdot))^{-1}$ are Lipschitz continuous over $U \times \Omega \times \Omega$, i.e., there exist constants $\ell_\nu^u, \ell_\nu^y, \tilde{\ell}_\nu^u$ such that for any $(y^1, u^1), (y^2, u^2) \in U \times \Omega \times \Omega$, we have

$$\begin{aligned} \|J_u \Phi_\nu(y^1, u^1) - J_u \Phi_\nu(y^2, u^2)\| &\leq \ell_\nu^u \|(y^1, u^1) - (y^2, u^2)\|, \\ \|J_y \Phi_\nu(y^1, u^1) - J_y \Phi_\nu(y^2, u^2)\| &\leq \ell_\nu^y \|(y^1, u^1) - (y^2, u^2)\|, \\ \|(J_u \Phi_\nu(y^1, u^1))^{-1} - (J_u \Phi_\nu(y^2, u^2))^{-1}\| &\leq \tilde{\ell}_\nu^u \|(y^1, u^1) - (y^2, u^2)\|. \end{aligned}$$

Moreover, there exists $M_\ell > 0$ such that $\ell_\nu^u \leq \frac{M_\ell}{\nu}$ and $\ell_\nu^y \leq \frac{M_\ell}{\nu}$.

(vi) Assume that $\tau\gamma < 1$ and $\gamma > L_Q$, where L_Q is the Lipschitz constant of ∇Q_μ over $U \times \Omega$. Given any $\nu \in [0, 1]$ and $\tilde{y} \in U \times \Omega$,

$$\|\Phi_\nu(\tilde{y}, u^1) - \Phi_\nu(\tilde{y}, u^2)\| \geq \tau(\gamma - L_Q)\|u^1 - u^2\|$$

for any $u^1, u^2 \in \Omega$.

Proof. The continuous differentiability of Φ_ν is due to Lemma 7.1. Conclusion (i) is a simple consequence of Lemma 7.1(i), and conclusion (ii) is from the gradient consistency of smoothing functions.

(iii) Given any $\tilde{y} \in \mathbb{R}_+^r \times \Omega$, we have $J_u \phi(\tilde{y}, \tilde{u}) = \gamma I_q + \nabla_u^2 Q_\mu(\tilde{w}; \tilde{\lambda})$ for any $\tilde{u} \in \Omega$. From [16, Proposition 2.3.2], $\phi(\tilde{y}, \cdot)$ is strongly monotone over Ω . By virtue of a proof similar to that of [8, Proposition 4.2] and Lemma 7.1(iii), we can obtain the conclusion.

(iv) From the compactness of $U \times \Omega \times \Omega$, we can find that $J_u \Phi_\nu$ and $J_y \Phi_\nu$ are bounded over $U \times \Omega \times \Omega$. Bounds b^u and b^y are not related to ν because of Lemma 7.1(iii). Now we prove the boundedness of $(J_u \Phi_\nu(\cdot, \cdot))^{-1}$. Let $A = J_u \Phi_\nu(\tilde{y}, \tilde{u})$. Using [21, Example 5.6.6], we can prove that

$$\|A^{-1}\| = \frac{1}{\sigma_q(A)} \leq \frac{(\sigma_1(A))^{q-1}}{\sigma_1(A) \cdots \sigma_q(A)} = \frac{\|A\|^{q-1}}{|\det(A)|},$$

where $\sigma_k(A)$, $k = 1, \dots, q$, denotes the k -th largest singular value of A . Since $U \times \Omega \times \Omega$ is compact, there exists some $(\hat{y}, \hat{u}) \in U \times \Omega \times \Omega$ such that $|\det(J_u \Phi_\nu(\hat{y}, \hat{u}))| \leq |\det(J_u \Phi_\nu(\tilde{y}, \tilde{u}))|$ for any $(\tilde{y}, \tilde{u}) \in U \times \Omega \times \Omega$. Denote $\tilde{b}_\nu^u := \frac{(b^u)^{q-1}}{|\det(J_u \Phi_\nu(\hat{y}, \hat{u}))|}$. Noting that b^u is the upper bound for $\|J_u \Phi_\nu(\cdot, \cdot)\|$, we have $\|(J_u \Phi_\nu(\tilde{y}, \tilde{u}))^{-1}\| \leq \tilde{b}_\nu^u$ for $(\tilde{y}, \tilde{u}) \in U \times \Omega \times \Omega$. Then we prove the other conclusion. Let $g(\tilde{y}, \tilde{u}, \nu) = |\det(J_u \Phi_\nu(\tilde{y}, \tilde{u}))|$ for $(\tilde{y}, \tilde{u}, \nu) \in U \times \Omega \times \Omega \times [\tilde{c}, 1]$. From the definition of $\varphi_\nu(t)$ in (7.1), we know that g is continuous over compact set $U \times \Omega \times \Omega \times [\tilde{c}, 1]$. So there exists $(\hat{y}, \hat{u}, \hat{\nu}) \in U \times \Omega \times \Omega \times [\tilde{c}, 1]$ such that $0 < g(\hat{y}, \hat{u}, \hat{\nu}) \leq g(\tilde{y}, \tilde{u}, \nu)$ for any $(\tilde{y}, \tilde{u}, \nu) \in U \times \Omega \times \Omega \times [\tilde{c}, 1]$. Denote $\tilde{b}^u := \frac{(b^u)^{q-1}}{|\det(J_u \Phi_\nu(\hat{y}, \hat{u}))|}$. Then we have $\|(J_u \Phi_\nu(\tilde{y}, \tilde{u}))^{-1}\| \leq \tilde{b}^u$ for $(\tilde{y}, \tilde{u}) \in U \times \Omega \times \Omega$ and $\nu \in [\tilde{c}, 1]$.

(v) From Lemma 7.1(iii)(iv)(v) and the compactness of $U \times \Omega \times \Omega$, we can find that $J_u \Phi_\nu$ and $J_y \Phi_\nu$ are Lipschitz continuous over $U \times \Omega \times \Omega$, and constant $M_\ell > 0$

697 is constructed from M^i in Lemma 7.1(v). Thus it suffices to prove that $(J_u \Phi_\nu(\cdot, \cdot))^{-1}$
 698 is Lipschitz continuous over $U \times \Omega \times \Omega$. Let $J_u^k = J_u \Phi_\nu(y^k, u^k)$, $k = 1, 2$. Actually,

$$\begin{aligned} \|(J_u^1)^{-1} - (J_u^2)^{-1}\| &= \|(J_u^2)^{-1}(J_u^1 - J_u^2)(J_u^1)^{-1}\| \\ &\leq \|(J_u^2)^{-1}\| \|J_u^1 - J_u^2\| \|(J_u^1)^{-1}\| \\ &\leq (\tilde{b}_\nu^u)^2 \ell_\nu^u \|(y^1, u^1) - (y^2, u^2)\|. \end{aligned}$$

700 Letting $\tilde{\ell}_\nu^u := (\tilde{b}_\nu^u)^2 \ell_\nu^u$, we can prove the conclusion.

701 (vi) We firstly show that the conclusion holds with $\nu = 0$. Actually, from $\Phi_0 = \Phi$,
 702 we have

$$\begin{aligned} &\|\Phi(\tilde{y}, u^1) - \Phi(\tilde{y}, u^2)\| \\ &\geq \|u^1 - u^2\| - \|\Pi_\Omega(u^1 - \tau\phi(\tilde{y}, u^1)) - \Pi_\Omega(u^2 - \tau\phi(\tilde{y}, u^2))\| \\ &\geq \|u^1 - u^2\| - \|(u^1 - \tau\phi(\tilde{y}, u^1)) - (u^2 - \tau\phi(\tilde{y}, u^2))\| \\ &\geq \|u^1 - u^2\| - (1 - \tau\gamma + \tau L_Q) \|u^1 - u^2\| \\ &= \tau(\gamma - L_Q) \|u^1 - u^2\|, \end{aligned}$$

704 where the second inequality follows from Lemma 7.2(i). For the case that $\nu > 0$, from
 705 Lemma 7.1(iii), note that $\|\Psi_\nu(\tilde{y}, u^1) - \Psi_\nu(\tilde{y}, u^2)\| \leq \|u^1 - u^2\|$ for any $u^1, u^2 \in \mathbb{R}^q$.
 706 Hence, the conclusion for $\nu > 0$ can be proved similarly. \square