Abstract

The task of approximating an arbitrary convex function arises in several learning problems such as convex regression, learning with a difference of convex (DC) functions, and approximating Bregman divergences. In this paper, we show how a broad class of convex function learning problems can be solved via a 2-block ADMM approach, where updates for each block can be computed in closed form. For the task of convex Lipschitz regression, we establish that our proposed algorithm converges with iteration complexity of $O(n\sqrt{d}/\epsilon)$ for a dataset $X \in \mathbb{R}^{n \times d}$ and $\epsilon > 0$. Combined with per-iteration computation complexity, our method converges with the rate $O(n^3d^{1.5}/\epsilon + n^2d^{2.5}/\epsilon + nd^3/\epsilon)$. This new rate improves the state of the art rate of $O(n^5d^2/\epsilon)$ available by interior point methods if $d = o(n^4)$. Further we provide similar solvers for DC regression and Bregman divergence learning. Unlike previous approaches, our method is amenable to the use of GPUs. We demonstrate on regression and metric learning experiments that our approach is up to 30 times faster than the existing method, and produces results that are comparable to state-of-the-art.

1 INTRODUCTION

Convex regression is the problem of estimating a convex function when receiving a dataset $\{(x_i, y_i)\}_{i=1}^n$, where $x_i \in \mathbb{R}^d$ are predictors and $y_i$ are continuous responses. Consider

$$\mathcal{F} \triangleq \{ f : \mathbb{R}^d \to \mathbb{R} \mid f \text{ is convex} \},$$

be the class of all convex functions over $\mathbb{R}^d$. Then an estimator is proposed by minimizing the squared error between observations $x_i$ and response $y_i$,

$$f \triangleq \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \| f \|,$$

where $\| f \|$ is a penalty term.

Although Eq. (2) is an infinite dimensional minimization problem, Boyd et al. (2004) shows it can be solved as a convex optimization problem. Generalization bounds for this problem are provided in (Balázs 2016; Siahkamari et al. 2020) using certain classes for $\| f \|$. Hence one can provide an arbitrarily good approximation of any convex function given a large enough sample size. The downside is the computational complexity which is prohibitive for real applications.

Convex regression is used commonly in econometrics and engineering for modeling demand, utility and production curves (Afriat, 1967; Varian, 1982). Furthermore recently Siahkamari et al. (2019, 2020) used convex regression to learn a Bregman divergence for metric learning and difference of convex functions for a general piecewise linear estimator. More generally, problems involving learning convex functions arise frequently in machine learning. Neural network-based methods have been proposed to learn convex functions and have been applied to tasks such as image completion and reinforcement learning (Amos et al. (2017)). Similarly, convex function learning has been applied to the problem of learning a convex function to parameterize an $f$-divergence for the task of imitation learning (Zhang et al. (2020)). Recently, a generalization of Mahalanobis metric learning has been studied, where one learns an arbitrary Bregman divergence based on supervision; such divergences are parameterized by a strictly convex function, leading to a learning problem over the space of strictly convex functions (Siahkamari et al. (2019)). Further, generalization of the convex regression problem to the setting where we learn a difference of two convex functions; has been studied. Such a class is very rich, containing all $C^2$ functions (Siahkamari et al. (2020)).
In this paper we provide an iterative 2-block ADMM algorithm for the convex regression problem, which we denote as the Faster Convex Regression (FCR) solver. Each block of FCR consists of closed form solutions, and it is guaranteed to converge with computational complexity of $O(n^3 d^{1.5} / \epsilon + n^2 d^{2.5} / \epsilon + n d^3 / \epsilon)$ for a dataset $X \in \mathbb{R}^{n \times d}$ and $\epsilon > 0$. This new rate improves the state of the art $O(n^2 d^2)$ available via interior point methods when $d = o(n^3)$. In addition to an improved convergence rate, FCR makes several contributions. Firstly, FCR is stand-alone and does not need any optimization software. FCR is based on tensor computations and can easily be implemented on GPUs. Secondly, FCR can include regularization terms in the context of the non-parametric convex regression. In this paper, we use the equivalent of $L_1$ for feature sparsity to improve interpretability and reduce over-fitting in higher dimensional datasets. Lastly, we extend the FCR solver for problems beyond convex Lipschitz regression. In particular, we provide 2-block ADMM solvers and empirical comparisons for difference of convex functions, (DC) regression [Siahkamari et al., 2020] and Bregman divergence learning [Siahkamari et al., 2019].

Notation. We generally denote scalars as lower case letters, vectors as lower case bold letters, and matrices as upper case bold letters. For a dataset $X \in \mathbb{R}^{n \times d}$, $n$ represents the number of observations and $d$ is the number of covariates. We define $x^+ = \max(x, 0)$, $x^- = \max(-x, 0)$ and $x$ as an outer product. We define $[n]$ to be the set of integers \{1, \ldots, n\}.

1.1 Connections to Existing Methodologies

Convex regression has been extensively studied over the last two decades. Boyd et al. (2004) introduced the non-parametric convex regression problem Eq. (2). Balázs (2016) showed that convex Lipschitz regression requires regularization in order to have generalization guarantees. That is, the penalty term $\|f\| = \sup_x \|\nabla f(x)\|$ results in a generalization error of $O(n^{-2/3} \log n)$.

Balázs (2016); Mazumder et al. (2019) provide ADMM solvers for the convex regression problem; however, solutions have more than two blocks and are not guaranteed to converge in all circumstances. More recently, Chen and Mazumder (2020) provided an active-set type solver and Bertsimas and Mundru (2021) provided a delayed constraint generation algorithm which have favorable scalability. They use a penalty of $\|f\| = \sum_i \|\nabla f(x_i)\|^2_2$, which makes the loss function in Eq. (2) strongly convex and easier to solve. However, no theoretical generalization bound is known when using this new penalty term. Siahkamari et al. (2020) uses $\|f\| = \sup_x (\|\nabla f(x)\|_1)$ for learning divergence of convex functions where they provide multi-block ADMM solver for this problem.

On the other hand, Ghosh et al. (2019) and Kim et al. (2021) study the parametric class of max-linear functions $F_k = \{f: \mathbb{R}^d \to \mathbb{R} \mid f(x) = \max_{j=1}^k (a_j, x) + b_j\}$ for $k < n$. They provide convex programming and alternating algorithms. The downside of these methods is the assumption that $x_i$ are i.i.d samples from a normal distribution and furthermore each feature $x_{i,t}$ is independent. These assumptions are needed for their algorithm to converge in theory. We note that this parametric class $F_k$ if $k \geq n$, is the same as $F$, when used in convex regression minimization problem Eq. (2).

Our methodology is most similar to Balázs (2016) and is in the context of learning theory where we do not require any distributional assumption on $x_i$ and only require them be i.i.d. and bounded. We further need to know a bound on $f$ and not on $\|f\|$.

2 Convex regression with Lasso penalty

Given a dataset $\{(y_i, x_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$ are predictors, assumed drawn i.i.d. from a distribution $P_X$ supported on a compact domain $\Omega \subset \{\|x\| \leq L\}$, with $n \geq d$, and $y_i$ are responses such that $y_i = f(x_i) + \varepsilon_i$ for a centered, independent random noise $\varepsilon_i$. Assume $|\varepsilon_i|$ and $|f(\cdot)|$ both are bounded by $M$. Furthermore $f$ is convex and Lipschitz. We propose to solve the penalized convex regression problem in Eq. (2) with the penalty term $\|f\| = \frac{1}{n} \sum_{i=1}^n \sup_x \|\partial_{x_i} f(x)\|$ This would result in the following convex optimization problem:

$$\min_{\hat{y}, \hat{x}} \frac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_i)^2 + \lambda \sum_{i=1}^d \max_{i=1}^n |a_{i,l}|$$

s.t. $\hat{y}_i - \hat{y}_j - \langle a_i, x_i - x_j \rangle \leq 0 \quad i, j \in [n] \times [n]$. Then, we estimate $f(x)$ via

$$\hat{f}(x) = \max_{i} (a_i, x - x_i) + \hat{y}_i. \quad (4)$$

This is a model similar to Balázs (2016) with a minor modification of using a different penalty term in the loss function. Our penalty term depends on the sum of partial derivatives $\sum_{i=1}^d \sup_x \|\partial_{x_i} f(x)\|$ rather than $\sup_x \|\nabla f(x)\|_2^2$. This new penalty term acts similar to a $L1$ regularizer and encourages feature sparsity. It is easy to show the estimator is bounded i.e., $\sup_{x \in \Omega} \|f(x)\| \leq M + 4 \|f\|_{\mathcal{F}}$. Also $\|f + g\| \leq \|f\| + \|g\|$, $\|f\| = c \|f\|$ for $c \geq 0$. Hence similar to Siahkamari et al. (2020) our penalty term is a valid seminorm which utilizes us to use their theorem here.
Proposition 1. With the appropriate choice of $\lambda$ which requires knowledge of $M$ the bound on $f$ and $n \geq d$, it holds that with probability at least $1 - \delta$ over the data, the estimator $\hat{f}$ of (4) excess risk is upper bounded by
\[
\mathbb{E}[|f(x) - \hat{f}(x)|^2] \leq O \left( \frac{n}{d} \sqrt{\frac{r^2}{d}} \log \left( \frac{n}{d} \right) + \sqrt{\frac{\log(1/\delta)}{n}} \right).
\]

2.1 Optimization

Our method utilizes well known ADMM (Gabay and Mercier 1976) algorithm. ADMM is a standard tool for solving convex problems that consists of two variable blocks with linear constraints (Eckstein and Yao 2012). It has an iterative procedure to update the problem variables with provable convergence guarantees (He and Yuan 2012).

We solve program (3) using ADMM. We first consider an equivalent form of the optimization problem as:
\[
\min_{\hat{y}_i, a_i, L_i \geq 0} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 + \lambda \sum_{i=1}^{d} L_i \tag{5}
\]
\[
\text{s.t. } \left\{ \begin{array}{l}
\sum_{i=1}^{n} p_i^+ - \sum_{i=1}^{n} p_i^- = 0, \\
\sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j} (\hat{y}_i - \hat{y}_j - \langle a_{i,j}, x_i - x_j \rangle) = 0, \\
\sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j} (\hat{y}_i - \hat{y}_j - \langle a_{i,j}, x_i - x_j \rangle) = 0, \\
\sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j} (\hat{y}_i - \hat{y}_j - \langle a_{i,j}, x_i - x_j \rangle) = 0.
\end{array} \right. \tag{6}
\]

with the augmented Lagrangian
\[
\ell(\hat{y}_i, a_i, L_i, p_i^+, p_i^-, u_i, s_{i,j}) = -\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 + \lambda \sum_{i=1}^{d} L_i
\]
\[
+ \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\rho}{2} (s_{i,j} + \hat{y}_i - \hat{y}_j - \langle a_{i,j}, x_i - x_j \rangle + \alpha_{i,j})^2
\]
\[
+ \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\rho}{2} (u_{i,l} + p_{i,l}^+ - p_{i,l}^- - L_i + \gamma_{i,l})^2
\]
\[
+ \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\rho}{2} (a_{i,l} - p_{i,l}^+ + p_{i,l}^- + \eta_{i,l})^2,
\]

where $\alpha_{i,j}$, $\gamma_{i,l}$ and $\eta_{i,l}$ are dual variables. We divide parameters into two blocks as $b^1 = \{\hat{y}_i, a_i\}$ and $b^2 = \{L_i, p_i^+, p_i^-, u_i, s_{i,j}\}$, where $i,j \in [n] \times [n], l \in [d]$. We find closed form solutions for each block given the solution to the other block.

2.1.1 First block $b^1 = \{\hat{y}_i, a_i\}$

We first note that we always normalize the dataset such that $\sum_{i=1}^{n} x_i = 0$ and $\sum_{i=1}^{n} y_i = 0$. This will result in $\sum_{i=1}^{n} \hat{y}_i = 0$ and simplify the solutions.

By setting $\nabla_{a_i} \ell = 0$ we can solve for $a_i$ as:
\[
a_i = \Lambda_i (\theta_i + \hat{y}_i x_i + \frac{1}{n} \sum_{k=1}^{n} \hat{y}_k x_k), \tag{6}
\]

where
\[
\Lambda_i \triangleq (x_i x_i^T + \frac{1}{n} I + \frac{1}{n} \sum_j x_j x_j^T)^{-1},
\]
\[
\theta_i \triangleq \frac{1}{n} (p_i^+ - p_i^- - \eta_i + \sum_j (\alpha_{i,j} + s_{i,j})(x_i - x_j)).
\]

Similarly by setting $\partial_{y_i} \ell = 0$ and substituting Eq. (6) for $a_i$, we can solve for $\hat{y}_i$. It is easy to find the solution to this problem w.r.t. $L_i$, using a sort and a simple algorithm that takes $O(n \log n)$ flops; see - L_update- algorithm (1). Observe that it is possible to add monotonous constraints for $\hat{f}$ by projecting either $p_{i,l}^+$ or $p_{i,l}^-$ to zero.
Algorithm 1 L-update

Require: \{\gamma_i, c_i\}_{i=1}^n, and \rho/\lambda
1: knot_{2n}, \ldots, knot_1 \leftarrow \text{sort}\{\gamma_i + c_i, \gamma_i - c_i\}_{i=1}^n
2: f \leftarrow \lambda/\rho
3: f' \leftarrow 0
4: for \ j = 2 \ to \ 2n \ do
5: \quad f' \leftarrow f' + \frac{1}{2}
6: \quad f \leftarrow f + f' \cdot (\text{knot}_j - \text{knot}_{j-1})
7: \quad if \ f \leq 0 \ then
8: \quad \quad \text{return} \ (\text{knot}_j - \frac{f}{T})^+
9: \quad \text{end if}
10: \text{end for}
11: \text{return} \ (\text{knot}_{2n} - \frac{f}{T})^+

Algorithm 2 Convex regression

Require: \{(x_i, y_i)\}_{i=1}^n, \rho, \lambda, \text{and } T
1: \hat{y}_i = s_{i,j} = 0i,j
2: L = a_i = p_i = u_i = \eta_i = \gamma_i \leftarrow 0_{d \times 1}
3: for \ t = 1 \ to \ T \ do
4: \quad \text{Update } \hat{y} \text{ by Eq. } (7)
5: \quad \text{Update } a_i \text{ by Eq. } (6)
6: \quad L_i \leftarrow L \text{-update}(\{\hat{\gamma}_i, \eta_{i,l}\}_{i\in[n]}, \lambda/\rho)
7: \quad \text{Update } u_{i,l}, p_{i,l}, \hat{p}_{i,l}, s_{i,j} \text{ by Eq. } (8)
8: \quad \text{Update } a_{i,j}, \hat{\gamma}_i, \eta_{i,l} \text{ by Eq. } (9)
9: \text{end for}
10: \text{return} \ f(\cdot) \triangleq \max_{i=1}^n (\langle a_i, \cdot \rangle - x_i) + \hat{y}_i

2.1.3 Dual variables

The update for dual variables follows from the standard ADMM algorithm updates:

\[
\alpha_{i,j} = \alpha_{i,j} + s_{i,j} + \hat{y}_i - \hat{y}_j - \langle a_i, x_i - x_j \rangle \quad i,j \in [n] \times [n]
\]

\[
\gamma_{i,l} = \gamma_{i,l} + u_{i,l} + \hat{p}_{i,l} + \hat{p}_{i,l} - L_i \quad i,l \in [n] \times [d]
\]

\[
\eta_{i,l} = \eta_{i,l} + a_{i,l} - p_{i,l} + \hat{p}_{i,l} \quad i,l \in [n] \times [d].
\]

2.1.4 Algorithms via ADMM

Algorithm 2 provides the full steps for a parallel ADMM optimizer for the convex regression problem. In each line in algorithm 2 we use subscripts such as \(i, j\) and \(l\) on the left hand side. These updates may be run in parallel for \(i \in [n], i,j \in [n] \times [n], i,l \in [n] \times [d]\) or \(q \in [2]\). We initially set all block variables to zero and normalize the dataset such that \(\sum_i y_i = 0\) and \(\sum_i x_i = 0\). We have implemented our algorithm using PyTorch [Paszke et al., 2019] which benefits from this parallel structure when using a GPU. Our code along with a built-in tuner for our hyperparameter \(\lambda\) and \(T\) is available on our GitHub repository [1].

2.2 Analysis

Our method has two sources of errors which are the error due to the ADMM procedure (Eq. 5) and the error due to the estimating ground truth convex function (Eq. 6). We characterize both errors based on ADMM convergence [He and Yuan (2012)].

**Theorem 1.** ([from He and Yuan (2012)] Consider the separable convex optimization problem,

\[
\min_{b_1 \in S_1, b_2 \in S_2} [\psi(b_1, b_2) = \psi_1(b_1) + \psi_2(b_2)]
\]

\[s.t.: Ab_1 + Bb_2 + b = 0,\]

where \((b_1, b_2)\) are the block variables, \((S_1, S_2)\) are convex sets, \((A, B)\) are the coefficient matrices and \(b\) is a constant vector. Let \(b_1^\ast\) and \(b_2^\ast\) be solutions at iteration \(t\) of a two block ADMM procedure with learning rate \(\rho\) starting from all zero vectors. Denote average of iterates as \(\hat{b}_1^t, \hat{b}_2^t = \frac{1}{T} \sum_{t=1}^T b_1^t, \frac{1}{T} \sum_{t=1}^T b_2^t\). For all \(\kappa\) we have,

\[
\psi(\hat{b}_1^t, \hat{b}_2^t) - \psi(b_1^\ast, b_2^\ast) - \kappa^T(A\hat{b}_1^t + B\hat{b}_2^t + b)
\]

\[
\leq \frac{1}{T} \left( \frac{\rho}{2} \|B\hat{b}_2^t\|^2 + \frac{1}{2\rho} \|\kappa\|^2 \right),
\]

where \((b_1^\ast, b_2^\ast)\) are the optimal solutions.

We arranged Theorem 1 such that it explicitly depends on the problem dependent constants such as \(\|B\hat{b}_2^t\|^2\), the number of iterations, \(T\), as well as the learning rate \(\rho\). A shorter proof for the case where \(S_1\) and \(S_2\) are the real coordinate space is provided in Appendix A.1

Next, we present convergence analysis in terms of regularized MSE of the output of the ADMM algorithm [2]. This has the further benefit of finding an appropriate learning rate \(\rho\) and a range for regularization coefficient \(\lambda\) that minimizes the computational complexity.

**Theorem 2.** Let \(\{\hat{y}_i, a_i^t\}_{i=1}^n\) be the output of Algorithm 2 at \(t\)th iteration, \(\hat{y}_i \triangleq \frac{1}{T} \sum_{t=1}^T \hat{y}_i^t\) and \(\bar{a}_i \triangleq \frac{1}{T} \sum_{t=1}^T a_i^t\). Denote \(\hat{f}_T(x) \triangleq \max_{i} \langle \bar{a}_i, x - x_i \rangle + \hat{y}_i\). Assume \(\max_{i,l} |x_{i,l}| \leq 1\) and \(\text{Var}(\{y_i\}_{i=1}^n) \leq 1\). If we choose \(\rho = \frac{n d^2}{\sqrt{\text{Var}(\{y_i\}_{i=1}^n)}}\), for \(\lambda \geq \frac{\sqrt{\text{Var}(\{y_i\}_{i=1}^n)}}{\sqrt{2nd}}\) and \(T \geq 2nd\) we have:

\[
\frac{1}{n} \sum_{i=1}^n (\hat{f}_T(x_i) - y_i)^2 + \lambda \|f\|^2
\]

\[
\leq \min_{f \in \mathcal{F}} \left( \frac{1}{n} \sum_{i=1}^n (\hat{f}(x_i) - y_i)^2 + \lambda \|f\|^2 \right) + 6n\sqrt{\frac{d}{T + 1}}.
\]

**Corollary 1.** Our method needs \(T = \frac{6n d^2}{\varepsilon}\) iterations to achieve \(\varepsilon\) error. Each iteration requires \(O(n^2d + nd^2)\) flops operations. Preprocessing costs \(O(nd^3)\). Therefore the total computational complexity is \(O(n^3d^5 + n^2d^2 + nd^3)\).

[1] Paszke et al., 2019

[2] He and Yuan (2012)
We note that assumptions of theorem \([2]\) are simply satisfied by normalizing the training dataset. The main difficulty for the derivation of theorem \([2]\) is: \((\hat{a}_i, \hat{y}_i)\) might be violating the constraints in \([5]\). This could result in \(\hat{f}_F(x_i) \neq \hat{y}_i\) and \(\|f\| \neq \sum_{i=1}^d L_i\). Therefore main steps of the proof of theorem \([2]\) is to characterize and bound the effect of such constraint violations on our objective function. Then setting \(\kappa\) theorem \([1]\) in a way to cover for the effects of constraint violations. For a proof we refer to Appendix A.2

3 Approximating a Bregman Divergence

We also consider the application of learning a Bregman divergence from supervision. This problem is a type of metric learning problem, where we are given supervision (pairs of similar/dissimilar pairs, or triplets consisting of relative comparisons amongst data points) and we aim to learn a task-specific distance or divergence measure from the data. Classical metric learning methods typically learn a linear transformation of the data, corresponding to a Mahalanobis-type distance function \(\|x\|_M = \sqrt{x^TMx}\). More generally, Mahalanobis distances are examples of Bregman divergences, which include other divergences such as the KL-divergence as special cases. Recent Siahkamari et al. (2019) formulated learning a Bregman divergence as learning the underlying convex function parameterizing the divergence. The resulting optimization problem they find is similar to convex regression problem Eq. \([5]\). Here we will discuss an improvement to their approach with a slightly different loss function and our Lasso penalty term. We derive an algorithm using 2-block ADMM. The existing solver for this problem uses standard linear programming.

In particular suppose we observe the classification dataset \(S_n = \{(x_i, y_i)\}_{i=1}^n\), for \(x_i \in \mathbb{R}^d\) and \(y_i\) is an integer. Let

\[
D_f(x_i, x_j) = f(x_i) - f(x_j) - \langle \nabla_x f(x_j), x_i - x_j \rangle,
\]

be a Bregman divergence with convex generating function \(f(x) \in \mathcal{F}\) and \(\nabla_x f(x)\) its largest sub-gradient. Let the pairwise similarity loss be

\[
\ell(D_f(x_i, x_j), y_i, y_j) = 1[y_i = y_j] - (D_f(x_i, x_j) \geq 1).
\]

We estimate \(f\) the underlying convex function of the Bregman divergence \(D_f\) by,

\[
\hat{f} \triangleq \arg\min_{f \in \mathcal{F}} \sum_{i=1}^n \sum_{j=1}^n \ell(D_f(x_i, x_j), y_i, y_j) + \lambda\|f\|.
\]

3.1 Optimization

In this section we provide an algorithm for the Bregman divergence learning based on 2block ADMM. We solve for each block in closed form. We first re-formulate the optimization problem to standard form and introducing some auxiliary variables we have:

\[
\begin{align*}
\min_{z_i, a_i, \nu_i, s_i, t_i, j} & \quad \sum_{i=1}^n \sum_{j=1}^n \zeta_{i,j} + \lambda \sum_d L_d \\
\text{s.t.} & \quad t_{i,j} s_{i,j} - t_{i,j} + t_{i,j} + 1 - \zeta_{i,j} = 0, i, j \in [n] \times [n] \\
& \quad s_{i,j} + z_i - z_j - (a_i, x_i - x_j) = 0, i, j \in [n] \times [n] \\
& \quad p_{i,l}^+ + p_{i,l}^- + u_{i,l} - L_l = 0, i, l \in [n] \times [d] \\
& \quad a_i, f \triangleq (2 - x_i^T A_i x_i) 1[i = j] - \frac{1}{n} D_{i,j}.
\end{align*}
\]

Now we write the augmented Lagrangian:

\[
\ell(z_i, a_i, \zeta_{i,j}, L_l, p_{i,j}^+, p_{i,j}^-, u_i, s_i, t_i, j)
\]

\[
= \sum_{i=1}^n \sum_{j=1}^n \zeta_{i,j} + \lambda \sum_d L_d \\
+ \sum_{i=1}^n \sum_{j=1}^n \rho \left( s_{i,j} + z_i - z_j - (a_i, x_i - x_j) + \alpha_{i,j} \right)^2 \\
+ \sum_{i=1}^n \sum_{l=1}^d \rho \left( u_{i,l} - p_{i,l}^+ + p_{i,l}^- - L_l + \gamma_{i,l} \right)^2 \\
+ \sum_{i=1}^n \sum_{j=1}^n \rho \left( a_i, f \triangleq (2 - x_i^T A_i x_i) 1[i = j] - \frac{1}{n} D_{i,j} \right)^2,
\]

where \(\alpha_{i,j}, \gamma_{i,j}, \eta_{i,j}\) and \(\tau_{i,j}\) are dual variables. Next we divide the variables into two blocks and solve for each in closed form.

3.1.1 First block \(b^1 = \{z_i, a_i, \zeta_{i,j}\}\)

Setting \(\partial_{\zeta_{i,j}} \ell = 0\) gives:

\[
\zeta_{i,j} = \left( - \frac{1}{n \rho} + \tau_{i,j} + t_{i,j} s_{i,j} - t_{i,j} + t_{i,j} + 1 \right)^+.
\]

Collecting the terms containing \(a_i\) in Eq.\([10]\) and comparing to those in Eq. \([5]\), the solution for \(a_i\) follows:

\[
a_i \triangleq \Lambda_i (\theta_i + z_i x_i + \frac{1}{n} \sum_k z_k x_k).
\]

Set \(\partial_z \ell = 0, \sum_i z_i = 0\) and \(\sum_i x_i = 0\). Using Eq. \([10]\) we can solve for \(z_1, \ldots, z_n\) as

\[
z = \Omega^{-1}_b (\nu - \beta),
\]

where \(\Omega_{breg, i,j} = (2 - x_i^T A_i x_i) 1[i = j] - \frac{1}{n} D_{i,j}\).
Algorithm 3 Learning a Bregman divergence

1: Require: \( \{(x_i, y_i) \mid x_i \in \mathbb{R}^d, y_i \in \mathbb{N}\}_{i \in [n]} \) and \( \{\rho, \lambda, T\} \)
2: \( z_i = s_{i,j} = t_{i,j} = \alpha_{i,j} = \tau_{i,j} \leftarrow 0 \)
3: \( L = a_i = p_i = u_i = \eta_i = \gamma_i \leftarrow 0 \)
4: for \( t = 1 \) to \( T \) do
5: \( \text{Update } \zeta_{i,j} \text{ by Eq. (11)} \)
6: \( \text{Update } z \text{ by Eq. (13)} \)
7: \( \text{Update } a_i \text{ by Eq. (12)} \)
8: \( L_i \leftarrow L \text{ update}(\{\gamma_{i,l}, \eta_{i,l} + a_i \mid \}_{i \in [n]}, \lambda/\rho) \)
9: \( \text{Update } s_{i,j}, t_{i,j} \text{ by Eq. (14)} \)
10: \( \text{Update } u_{i,l}, p_{i,l}, p_{i,l}^\perp \text{ by Eq. (8)} \)
11: \( \text{Update } \alpha_{i,j}, \gamma_{i,l}, \eta_{i,l} \text{ by Eq. (9)} \)
12: \( \text{Update } \tau_{i,j} \text{ by Eq. (15)} \)
end for
14: return \( f(\cdot) \triangleq \max_{i=1}^n (\langle a_i^1, \cdot - x_i \rangle + z_i) \)

3.1.2 Second block \( b^2 = \{L_i, p_i, u_i, s_{i,j}, t_{i,j}\} \)

Comparing Eq. (10) and Eq. (5), we find that \( L_i, p_i \) and \( u_i \) have the same solutions as in sec 2.1.2. Hence we only proceed to solve for \( s_{i,j} \) and \( t_{i,j} \). Set \( \partial_{t_{i,j}} f = \partial_{s_{i,j}} = 0 \). Some algebra gives:

\[
s_{i,j} = \frac{1}{2}(\pi_{1,i,j}^2 + t_{i,j} \pi_{1,i,j}^1 - t_{i,j} \pi_{1,i,j}^2 \pi_{1,i,j}^1), \quad (14)
\]
\[
t_{i,j} = (\pi_{1,i,j}^1 - \pi_{1,i,j}^2 s_{i,j}),
\]

where

\[
\pi_{1,i,j}^1 \triangleq -\pi_{1,i,j}^1 + t_{i,j} - 1 + \zeta_{i,j},
\pi_{1,i,j}^2 \triangleq -\pi_{1,i,j}^2 - \pi_{1,i,j} - z_i + s_{i,j} + \langle a_i, x_i - x_j \rangle.
\]

3.1.3 Dual variables

We only see a new constraint different from Eq. (5) with dual multiplier \( \tau_{i,j} \). The update is

\[
\tau_{i,j} = \tau_{i,j} + \pi_{1,i,j} + t_{i,j} + 1 - \zeta_{i,j}, \quad (15)
\]

3.1.4 Algorithms via ADMM

Algorithm 3 provides full-steps for solving the Bregman divergence learning problem.

4 Difference of Convex (DC) regression

In this section, we extend our convex regression solver to the difference of convex regression as studied in Siahkamari et al. (2020). DC are functions \( f \) that can be represented as \( f = \phi^1 - \phi^2 \) for a choice of two convex functions. DC functions are a very rich class - for instance, they are known to contain all \( \mathcal{C}^2 \) functions. DC regression has been studied in Cui et al. (2018);
and \( \hat{y}^2 \) solutions by solving a system of linear equations,
\[
\hat{y}' = \frac{(-1)^q+1}{2} (\Omega + \frac{2I}{n^2 \rho})^{-1} (\frac{4y}{n^2 \rho} - \beta^1 - \beta^2) + \frac{1}{2} (\Omega - \frac{2I}{n^2 \rho})^{-1} (v^1 - \beta^1 + v^2 - \beta^2)
\]
Algorithm 4 provides the full steps to solve the difference of convex regression problem.

## 5 Experiments

In this section we provide experiments on real datasets from the UCI machine learning repository. We compare our (DC)-regression algorithm with state of the art regression models. Then, we experiment with the Bregman divergence learning algorithm (PBDL) and compare against its predecessor (PBDL,0) as well as state of the art classification models. All results are reported either on the pre-specified train/test split or a 5-fold cross validation set based on instruction for each dataset. Our experiments code is available in our Github repository.

### 5.1 Models

For the purpose of comparisons, we first of all picked the previous (DC)-regression and PBDL algorithms. Furthermore, we picked two popular tree-based algorithms XGboost and Random Forest. We also picked Lasso as a baseline. According to the study done by Fernández-Delgado et al.(2014, 2019) Random Forest achieves the state of the art on most regression and classification tasks. More recently, XGBoost has been shown to achieve the state of the art on many real datasets and Kaggle.com competitions. The following is the specific of hyper-parameter tuning for each.

**DC-regression:** We choose \( \lambda \) from grid \( 10^{-3.3} \) by 5 fold cross validation. Then we do at most 2 more rounds of grid search around the optimal \( \lambda \) at the first round. We fix \( \rho = 0.01 \) and choose \( T \) by early stopping; whenever validation error improvements is less than \( 10^{-3} \) after \( n \) iteration of ADMM.

**PBDL:** We predict the classes using a 5 nearest neighbour scheme \( i_{\text{nearest}}(x) = \arg \min_i D_o(x, x_i) \). where \( D_o \) is learned Bregman divergence. Tuning \( \lambda \) is similar to DC-regression

**PBDL:0:** We used their code for Learning a Bregman divergence based on Groubi solvers. We used their built in parameter tuner for \( \lambda \) which is based on 5 fold cross validation.

**XGboost Regressor/Classifier:** \( \text{max} \_ \text{depth} \) and \( \text{learning} \_ \text{rate} \) is found by 5 fold cross validation over \( \{1, \ldots , 10\} \times \{0.05, 0.1, 0.5\} \). Other parameters set to default. From xgboost 1.6.0 package in Chen and Guestrin (2016).

**Random Forest Regressor/Classifier:** \( n \_ \text{features} \) is found by 5 fold cross validation over \( [d^{0.25}, d^{0.75}] \). From sklearn package in Pedregosa et al. (2011).

**Lasso:** We used the sklearn package builtin function LassoCV.

### 5.2 Regression datasets

We chose all regression datasets from UCI which have number of instances \( 10^3 \leq n \leq 10^4 \). These were about 30 datasets at the time of submission of this paper. We had to discard 16 of these datasets due to various reasons such as: 1. dataset not available, 2. synthetic or simulated data, 3. text datasets, 4. complex spatio-temporal datasets, 5. classification dataset. Some of these datasets have multiple target variables, therefore we report the out of sample \( R^2 \) results with a suffix for each target variable.

### 5.3 Classification datasets

We chose all datasets originally used in Siahkamari et al. (2019). Further, we include the abalone dataset which was too large for the previous PBDL algorithm. We use these datasets as multi-class classification problems. We report accuracy as well as the training run-time.

The pre-processing code for each dataset and our testing pipeline is available in our GitHub repository.

### 5.4 Computing infrastructure

For the (DC)-regression and PBDL algorithms we use a V100 Nvidia GPU processor with 11 gigabyte of GPU memory, and 4 cores of CPU. For all the other methods we use a 16 core CPU.

### 5.5 Results

**Regression:** For our regression experiments we present the out of sample \( R^2 \) on 22 datasets in figure 4. We observe our method despite having \( n \times d \) parameters, has similar performance to that of XG-boost and Random Forest. We further observe that for solar-flare and Parkinson datasets where other methods overfit, our algorithm is more robust and avoids overfitting. Maximum number of instances which we were able to experiment on with reasonable time is about \( 10^4 \) and is \( 10x \) larger than what Siahkamari et al. (2020) has experimented on.
Classification: For our classification experiments we present the accuracy in figure 2(left). We observe that our Bregman divergence Learning Algorithm (PBDL) as well as the original (PBDL_0) have similar performance to that of XGboost and Random Forest. We compare the logarithm of runtimes of all methods in figure 2(right). In terms of speed we are one average 30x faster than the original PBDL_0 algorithm. Also PBDL_0 failed to handle the Abalone dataset with n = 4177, where the new PBDL took less than a minute to finish one fit. We are still well slower than XGboost and Random Forest. However we only rely on a python script code vs an optimized compiled code. We note that the divergence function learned in PBDL can be further used for other tasks such as ranking and clustering.

6 Conclusion

In this paper we, studied the nonparametric convex regression problem with a L1 regularization penalty. we provided a solver for this problem and proved the iteration complexity be $6n\sqrt{d}/\epsilon$. The total computational complexity is $O(n^3d^{1.5}/\epsilon + n^2d^{2.5}/\epsilon + nd^3/\epsilon)$, which improves that of $O(n^5d^2/\epsilon)$ already known for this problem. Our solver could easily benefit from parallel computation and use GPUs. Finally we extended our solver to the problem of difference of convex (DC) regression and the problem of learning an arbitrary Bregman divergence. We provided comparisons to state of the art regression and classifications models.

7 Future work

In the one dimensional convex regression problem, due to ordering of $\mathbb{R}$, we only have $n$ constraints. This suggests that in general, we might only have $O(nd)$ active constraints. Balázs (2016); Mazumder et al. (2019); Bertsimas and Mundru (2021) use delayed constraint generation techniques to exploit this property. These techniques could also be used in our algorithm 2 to decrease the number of variables, i.e. $s_{i,j}$ and $\alpha_{i,j}$ which normally have to be updated at each ADMM iteration for $i,j \in [n] \times [n]$. One can also incorporate the farthest point clustering algorithm originally proposed in Gonzalez (1985) to cluster the data points and use $k < n$ linear functions for convex regression.
Figure 2: Classification (left) accuracy (right) log(runtime) for all fits on UCI datasets

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Appendix to ‘Faster Convex Lipschitz Regression via 2 blocks ADMM’

A Derivations

A.1 ADMM Convergence

Theorem 1 gives convergence of the ADMM procedure. We follow analysis similar to [He and Yuan (2012)] and give all steps for the sake of completeness. We first restate the convergence as follows:

**Theorem 1.** Consider the separable convex optimization problem:

$$\min_{b^1, b^2} \left[ \psi(b^1, b^2) = \psi_1(b^1) + \psi_2(b^2) \right]$$

s.t.: $A b^1 + B b^2 + b = 0,$

where $(b^1, b^2)$ are the block variables, $(A, B)$ are the coefficient matrices and $b$ is a constant vector. Let $b^1_t$ and $b^2_t$ be solutions at iteration $t$ of a two block ADMM procedure with learning rate $\rho$, i.e:

$$b^1_{t+1} = \arg\min_{b^1} \psi_1(b^1) + \frac{\rho}{2} \| A b^1 + B b^2_t + b - \frac{1}{\rho} d_t \|^2$$

$$b^2_{t+1} = \arg\min_{b^2} \psi_2(b^2) + \frac{\rho}{2} \| A b^1_{t+1} + B b^2 + b - \frac{1}{\rho} d_t \|^2$$

$$d_{t+1} = d_t - \rho (A b^1_{t+1} + B b^2_{t+1} + b),$$

where $b^1_0 = b^2_0 = d_0 = 0$.

Denote the average of iterates as $(\bar{b}^1_T, \bar{b}^2_T) = \left( \frac{1}{T} \sum_{t=1}^T b^1_t, \frac{1}{T} \sum_{t=1}^T b^2_t \right)$. For all $\kappa$ we have

$$\psi(\bar{b}^1_T, \bar{b}^2_T) - \psi(b^1, b^2) - \kappa^T (A \bar{b}^1_T + B \bar{b}^2_T + b) \leq \frac{1}{T} \left( \frac{\rho}{2} \| B b^2_t \|^2 + \frac{1}{2\rho} \| \kappa \|^2 \right),$$

where $(b^1, b^2)$ are the optimal solutions.

Before presenting the proof, we define a dual variable like sequence $\{\bar{d}_t\}_t$ with the update relation as $\bar{d}_{t+1} = d_t - \rho (A b^1_{t+1} + B b^2_t + b)$. The only difference between $\bar{d}_{t+1}$ and $d_{t+1}$ is due to $b^2_t$ and $b^2_{t+1}$. We have the following relation:

$$\bar{d}_{t+1} - d_{t+1} = \rho B (b^2_{t+1} - b^2_t). \tag{18}$$

First order conditions of ADMM updates give $\nabla \psi_1(b^1_{t+1}) = -\rho A^T (A b^1_{t+1} + B b^2_t + b - \frac{1}{\rho} d_t)$ and $\nabla \psi_2(b^2_{t+1}) = -\rho B^T (A b^1_{t+1} + B b^2_{t+1} + b - \frac{1}{\rho} d_t)$. Combining first order relations and the $\{\bar{d}_t\}_t$ update rule we get

$$\nabla \psi_1(b^1_{t+1}) = A^T \bar{d}_{t+1}; \quad \nabla \psi_2(b^2_{t+1}) = B^T \bar{d}_{t+1} + \rho B^T B (b^2_t - b^2_{t+1}). \tag{19}$$

**Theorem 1** is a direct conclusion of the following lemma.

**Lemma 1.** For all $b^1, b^2, \kappa$ we have,

$$\psi(b^1, b^2) - \psi(b^1_{t+1}, b^2_{t+1}) + \kappa^T (A b^1_{t+1} + B b^2_{t+1} + b) - \frac{1}{T} \sum_{t=1}^T \psi(b^1_{t+1}, b^2_{t+1}) + \kappa^T (A b^1 + B b^2 + b) + Z_t - Z_{t+1} \geq 0,$$

where $Z_t = \frac{\rho}{2} \| b^2 - b^2_t \|_{B^T B}^2 + \frac{1}{2\rho} \| \kappa - d_t \|^2$ and $\| x \|_M^2 = x^T M x$.

Let $b^1, b^2$ be $(b^1, b^2)$. By definition we have $A b^1 + B b^2 + b = 0$ which cancels an inner product. Rearranging and averaging over time gives

$$\psi(b^1_{t+1}, b^2_{t+1}) - \psi(b^1, b^2) - \kappa^T (A b^1_{t+1} + B b^2_{t+1} + b) \leq Z_t - Z_{t+1}$$

$$\frac{1}{T} \left( \sum_{t=0}^{T-1} \psi(b^1_{t+1}, b^2_{t+1}) \right) - \psi(b^1, b^2) - \kappa^T (A b^1_{t+1} + B b^2_{t+1} + b) \leq \frac{1}{T} \left( \sum_{t=0}^{T-1} Z_t - Z_{t+1} \right).$$
The RHS telescopes. Since $Z_t \geq 0$ we have $RHS \leq Z_0$. We lower bound LHS with Jensen Inq. as $\psi(\tilde{b}_T^1, \tilde{b}_T^2) \leq \frac{1}{T} \sum_{t=0}^{T-1} \psi(b_{t+1}^1, b_{t+1}^2)$. Combining LHS and RHS we get

$$\psi(\tilde{b}_T^1, \tilde{b}_T^2) - \psi(b_T^1, b_T^2) - \kappa^T (A b_T^1 + B b_T^2 + b) \leq \frac{1}{T} Z_0,$$

which is the statement in Theorem 1 assuming the initial variables are 0s.

We continue to prove Lemma 1. We start with convexity definition for both $\psi_1$ and $\psi$ as,

$$\psi_1(b^1) - \psi_1(b_{t+1}^1) - (b^1 - b_{t+1}^1)^T \nabla \psi_1(b_{t+1}^1) \geq 0; \quad \psi_2(b^2) - \psi_2(b_{t+1}^2) - (b^2 - b_{t+1}^2)^T \nabla \psi_2(b_{t+1}^2) \geq 0.$$

Summing the relations and plugging in Eq. 19 give,

$$\psi(b^1, b^2) - (b^1 - b_{t+1}^1)^T A^T \tilde{d}_{t+1} - (b^2 - b_{t+1}^2)^T B^T \tilde{d}_{t+1} - \rho (b^2 - b_{t+1}^2)^T B^T B(b^2 - b_{t+1}^2) \geq 0.$$

(20)

The update rule of $\tilde{d}$ gives $A b_{t+1}^1 + B b_{t+1}^2 + b + \frac{1}{\rho} (\tilde{d}_{t+1} - d_i) = 0$. Then for all $\kappa$, we have $(\kappa - \tilde{d}_{t+1})^T (A b_{t+1}^1 + B b_{t+1}^2 + b) = 0$. Adding such a term to $T_1$ does not change its value. After adding the zero inner product, we rearrange $T_1$ as

$$T_1 = \kappa^T (A b_{t+1}^1 + B b_{t+1}^2 + b) - \tilde{d}_{t+1}^T (A b_{t+1}^1 + B b_{t+1}^2 + b) + \rho (b^2 - b_{t+1}^2)^T B^T B(b^2 - b_{t+1}^2)$$

$$+ (\kappa - \tilde{d}_{t+1})^T (B b_{t+1}^2 - b_{t+1}^2) + \frac{1}{\rho} (\tilde{d}_{t+1} - d_i).$$

Plugging Eq. 19 in $Y_3$ gives $Y_3 = \frac{1}{\rho} (\kappa - \tilde{d}_{t+1})^T (d_{t+1} - d_i)$.

We use the following norm square relation and prove it at the end,

**Lemma 2.** For a symmetric $M = M^T$ we have,

$$(x - y)^T M (z - t) = \frac{1}{2} (\|x - t\|_M^2 - \|x - z\|_M^2) + \frac{1}{2} (\|y - z\|_M^2 - \|y - t\|_M^2).$$

Using Lemma 2 we get

$$Y_2 = \frac{1}{2} (\|b^2 - b_{t+1}^2\|_{B^T B}^2 - \|b^2 - b_{t+1}^2\|_{B^T B}^2) = \frac{1}{2} \|b_{t+1}^2 - b_{t+1}^2\|_{B^T B}^2$$

$$Y_3 = \frac{1}{\rho^2} (\|\kappa - d_i\|_I^2 - \|\kappa - d_{t+1}\|_I^2) + \frac{1}{\rho^2} (\|\tilde{d}_{t+1} - d_i\|_I^2 - \|\tilde{d}_{t+1} - d_i\|_I^2),$$

since $B^T B$ and $I$ are symmetric matrices.

We combine $Y_2$ and $Y_3$ as

$$\rho Y_2 + Y_3 = \frac{\rho}{2} (\|b^2 - b_{t+1}^2\|_{B^T B}^2 - \|b^2 - b_{t+1}^2\|_{B^T B}^2) + \frac{1}{2\rho} (\|\kappa - d_i\|_I^2 - \|\kappa - d_{t+1}\|_I^2)$$

$$- \frac{1}{2\rho} (\|\tilde{d}_{t+1} - d_i\|_I^2) \leq 0 \quad (\text{due to Eq. 18})$$

$$= 0 \quad (\text{due to Eq. 18})$$

Plugging it back to $T_1$,

$$T_1 = Y_1 + \rho Y_2 + Y_3 \leq Y_1 + \frac{\rho}{2} (\|b^2 - b_{t+1}^2\|_{B^T B}^2 - \|b^2 - b_{t+1}^2\|_{B^T B}^2) + \frac{1}{2\rho} (\|\kappa - d_i\|_I^2 - \|\kappa - d_{t+1}\|_I^2) \leq Y_1 + Z_t - Z_{t+1}.$$

(21)
Upper bounding $T_1$ term in Eq. 20 with Eq. 21 gives

$$\psi(b_1, b^2) - \psi(b^1_{t+1}, b^2_{t+1}) + \kappa^T(\Ab^1_{t+1} + \Bb^2_{t+1} + b) - \ddbar^T_{t+1}(\Ab^1 + \Bb^2 + b) + Z_t - Z_{t+1} \geq 0,$$

which is the statement in Lemma 1. □

**Proof of Lemma 2**

Expand RHS as

$$RHS = \frac{1}{2} (t^T Mt - 2x^T Mt - z^T Mz + 2x^T Mz) + \frac{1}{2} (z^T Mz - 2y^T Mz - t^T Mt + 2t^T My)$$

$$= -x^T Mt + x^T Mz - y^T Mz + t^T My$$

$$= (x - y)^T M(z - t).$$

We reach the LHS. □
A.2 Proof for Theorem 2 (computational complexity)

Theorem 2. Let \( \{ \tilde{y}_t, a_t \} \) be the output of Algorithm \( (2) \) at the \( t \)th iteration, \( \tilde{y}_t \triangleq \frac{1}{T} \sum_{i=1}^{T} y_t^i \) and \( a_t \triangleq \frac{1}{T} \sum_{i=1}^{T} a_t^i \). Denote \( f_T(x) \triangleq \max_i (a_i, x - x_i) + \tilde{y}_t \). Assume \( \max_{i,t} |x_{i,t}| \leq 1 \) and \( \nabla \{ y_1, \ldots, y_n \} \leq 1 \). If we choose \( \rho = \frac{\sqrt{n} \lambda^2}{n} \), for \( \lambda \geq 3 \sqrt{2} \) and \( T \geq n \sqrt{d} \) we have:

\[
\frac{1}{n} \sum_i (f_T(x_i) - y_i)^2 + \lambda \| f_T \| \leq \min_{f} \left( \frac{1}{n} \sum_i (f(x_i) - y_i)^2 + \lambda \| f \| \right) + \frac{6n \sqrt{d}}{T + 1}.
\]

For the proof, we make extensive use of Theorem\((1)\) which provides convergence rate of a general 2-block ADMM for a separable convex program with linear constraints

\[
\psi(b^1, b^2) = \psi_1(b^1) + \psi_2(b^2)
\]

(22) It guarantees for all \( \kappa \) the average solutions of a 2-block ADMM \((\tilde{b}_T^1, \tilde{b}_T^2)\) satisfies

\[
\psi(\tilde{b}_T^1, \tilde{b}_T^2) - \psi(b^1, b^2) - \kappa^T (A\tilde{b}_T^1 + B\tilde{b}_T^2 + b) \leq \frac{1}{T} \left( \frac{\rho}{2} \| Bb^2 \|^2 + \frac{1}{2\rho} \| \kappa \|^2 \right),
\]

(23) where \((b_1^*, b_2^*)\) are the optimal solutions of program \((22)\).

However in Eq\. (7) we are solving a specific version of program \((22)\) of the form

\[
\min_{y_t, a_t, p_t, L_t, s_{i,l} \geq 0, a_{i,l} \geq 0} \left[ \frac{1}{n} \sum_{i=1}^{n} (\tilde{y}_i - y_i)^2 + \lambda \sum_{l=1}^{d} L_l \right]
\]

(24) To match the notations between \((24)\) and \((22)\) denote the optimal/average ADMM solutions to program \((24)\) as

\[
\begin{align*}
  b_1^* &= (\tilde{y}_1, \ldots, \tilde{y}_n, a_{1,1}, a_{1,2}, \ldots, a_{n,d})^T \\
  b_2^* &= (L_1, \ldots, L_d, p_{1,1}, \ldots, p_{n,d}, u_{1,1}, \ldots, u_{n,d}, s_{1,1}, \ldots, s_{n,n})^T \\
  b_T^1 &= (\tilde{y}_1, \ldots, \tilde{y}_n, a_{1,1}, a_{1,2}, \ldots, a_{n,d})^T \\
  b_T^2 &= (\tilde{L}_1, \ldots, \tilde{L}_d, \tilde{p}_{1,1}, \ldots, \tilde{p}_{n,d}, \tilde{u}_{1,1}, \ldots, \tilde{u}_{n,d}, \tilde{s}_{1,1}, \ldots, \tilde{s}_{n,n})^T.
\end{align*}
\]

(25) Therefore the separable losses for the average iterates of ADMM for program \((24)\) are

\[
\psi_1(b_T^1) = \frac{1}{n} \sum_{i=1}^{n} (\tilde{y}_i - y_i)^2,
\]

(26) \[ \psi_2(b_T^2) = \lambda \sum_{l=1}^{d} L_l. \]

Note that convergence rate for \( \psi_1(b_T^1) + \psi_2(b_T^2) \) is available by setting \( \kappa = 0 \) in \((23)\). However this is not sufficient for convergence of our objective \( \frac{1}{n} \sum_i (f_T(x_i) - y_i)^2 + \lambda \| f_T \| \). The reason is \((b_T^1, b_T^2)\) might be violating the constraints in \((24)\). This could result in \( f_T(x_i) \neq \tilde{y}_i \) and \( \| f_T \| \neq \sum_{l=1}^{d} L_l \). Therefore main steps of the proof of Theorem \((2)\) is to characterize and bound the effect of such constraint violations on our objective function. Let us specify how much each linear constraint in program \((24)\) is violated,

\[
\begin{align*}
  \varepsilon_{1,i,l} &= -\tilde{s}_{i,l} + \tilde{y}_i - y_j - \langle a_{j,l}, x_i - x_j \rangle, \\
  \varepsilon_{2,i,l} &= \tilde{u}_{i,l} + |p_{i,l}| - \tilde{L}_l, \\
  \varepsilon_{3,i,l} &= \tilde{a}_{i,l} - \tilde{p}_{i,l}.
\end{align*}
\]

We break the proof to smaller parts by first providing some intermediate lemmas.
Lemma 3. \[ \psi(b_1^*, b_2^*) = \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2 + \lambda \sum_l L_l \leq 1 \]

Proof. Note that \( b_1 = b_2 = 0 \) is a feasible solution and \((\hat{y}_i, L_l)\) is the optimal solution. Also algorithm 2 normalizes the dataset such that \( \sum_{i=1}^n y_i = 0 \), therefore
\[
\psi(b_1^*, b_2^*) \leq \psi(0, 0)
\]
\[
\frac{1}{n} \sum_{i=1}^n y_i^2 = \text{Var} \{y_i\}_{i=1}^n \leq 1.
\]

Lemma 4. \[ \|Bb_2^*\|_2^2 \leq 18 \frac{n^2}{\lambda^2} \]

Proof. Since \( p_{i,l} \) is a feasible solution we have \( |p_{i,l}| \leq L_l \). We also have:
\[
0 \leq s_{i,j} = \hat{y}_i - \hat{y}_j - (a_j, x_i - x_j)
\]
(by constraints definitions)
\[
\leq (a_i - a_j, x_i - x_j)
\]
(convexity)
\[
\leq 2 \sum_l L_l |x_{i,l} + x_{j,l}|
\]
\[
\leq 4 \sum_l L_l
\]
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\leq 4 \sum_l L_l
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\leq 4 \sum_l L_l
\]

Arranging the constraints in (24) into \((n^2 + nd + nd)\) rows and separating the \( b_1^*, b_2^* \) coefficients as \( A \) and \( B \) in order we have:
\[
Ab_1^* + Bb_2^* = 0
\]
\[
Bb_2^* = [-s_{1,1}, \ldots, -s_{n,n}, 0_{1,1}, \ldots, 0_{n,d}, -p_{1,1}, \ldots, -p_{n,d}]^T.
\]

Taking the norm
\[
\|Bb_2^*\|_2^2 = \sum_{i,j} s_{i,j}^2 + \sum_{i,l} p_{i,l}^2
\]
\[
\leq n^2 (4 \sum_{l=1}^d L_l)^2 + n \sum_{l=1}^d L_l^2
\]
\[
\leq 18 \frac{n^2}{\lambda^2}
\]

Lemma 5. \[ 0 \leq \hat{f}_T(x_i) - \hat{y}_i \leq \max_j (\varepsilon_{i,j}^1) \]

Proof.
\[
\hat{y}_i \leq \hat{f}_T(x_i) = \max_j (a_j, x_i - x_j) + \hat{y}_j
\]
(Definition)
\[
= \max_j (\hat{y}_i - \hat{s}_{i,j} + \varepsilon_{i,j}^1)
\]
(\( \varepsilon_{i,j}^1 \) definition)
\[
\leq \hat{y}_i + \max_j (\varepsilon_{i,j}^1)
\]
(\( \hat{s}_{i,j} \geq 0 \))

Lemma 6.
\[
\frac{1}{n} \sum_i (\hat{f}_T(x_i) - y_i)^2 \leq \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2 + \frac{1}{n} \sum_j \max_j (\varepsilon_{i,j}^1)^2 + 2 \sqrt{\frac{1}{n} \sum_j \max_j (\varepsilon_{i,j}^1)^2} \sqrt{1 + \frac{9 \rho m^2}{T \lambda^2}}.
\]
Proof.

\[
\frac{1}{n} \sum_i (\hat{f}_T(x_i) - y_i)^2 = \frac{1}{n} \sum_i (\hat{f}_T(x_i) - \hat{y}_i + \hat{y}_i - y_i)^2
\]

\[
= \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2 + \frac{1}{n} \sum_i (\hat{f}_T(x_i) - \hat{y}_i)^2 + \frac{2}{n} (\hat{f}_T(x_i) - \hat{y}_i)(\hat{y}_i - y_i)
\]

\[
\leq \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2 + \frac{1}{n} \sum_i \max_j (\varepsilon_{i,j})^2 + \frac{2}{n} \max_j (\varepsilon_{i,j})(|\hat{y}_i - y_i|)
\]  \hspace{1cm} \text{(Lemma 5)}

Let us focus on the last term on the RHS.

\[
\left(\frac{1}{n} \sum_i \max_j (\varepsilon_{i,j})^2 |\hat{y}_i - y_i|\right)^2 \leq \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2
\]

\[
\leq \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2 + \lambda \sum_l \tilde{L}_l
\]  \hspace{1cm} \text{(\tilde{L}_l \geq 0)}

\[
\leq \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2 + \lambda \sum_l L_l + \frac{1}{T} \|Bb^2\|^2
\]  \hspace{1cm} \text{(Use Theorem 1 with \(\kappa = 0\))}

\[
\leq 1 + \frac{\rho}{T} \|Bb^2\|^2
\]  \hspace{1cm} \text{(Lemma 4)}

\[
\leq 1 + \frac{9\rho n^2}{T - \lambda^2}
\]  \hspace{1cm} \text{(Lemma 4)}

On the other hand for regularization term we have

**Lemma 7.** \(\|\hat{f}_T\| \leq \sum_l |\tilde{L}_l| + \sum_l \max_i |\varepsilon_{i,1}| + \max_i |\varepsilon_{i,3}^3|\).

Proof.

\[
\|\hat{f}_T\| = \sum_l \max_i |\tilde{a}_{i,l}|
\]

\[
= \sum_i \max_l |\tilde{b}_{i,l} + \varepsilon_{i,3}^3|
\]  \hspace{1cm} \text{(\varepsilon_{i,3}^3 definition)}

\[
\leq \sum_l |\tilde{L}_l| + \sum_i \max |\varepsilon_{i,1}^2| + \max |\varepsilon_{i,3}^3|
\]  \hspace{1cm} \text{(\varepsilon_{i,3}^3 definition)}

Next we combine the previous lemmas to prove Theorem 2. Before proceeding let's incorporate the definitions of constraint violations Eq. (27) in \(\kappa^T (Ab_1^T + Bb_2^2 + b)\) to get:

\[
\kappa^T (Ab_1^T + Bb_2^2 + b) = \kappa^1 \varepsilon^1 + \kappa^2 \varepsilon^2 + \kappa^3 \varepsilon^3,
\]  \hspace{1cm} \text{(28)}

where

\[
\kappa^1 \triangleq [\kappa^1_{1,1}, \ldots, \kappa^2_{n,n}]^T, \hspace{1cm} \kappa^2 \triangleq [\kappa^2_{1,1}, \ldots, \kappa^2_{n,d}]^T, \hspace{1cm} \kappa^3 \triangleq [\kappa^3_{1,1}, \ldots, \kappa^3_{n,d}]^T
\]

\[
\varepsilon^1 \triangleq [\varepsilon^1_{1,1}, \ldots, \varepsilon^2_{n,n}]^T, \hspace{1cm} \varepsilon^2 \triangleq [\varepsilon^2_{1,1}, \ldots, \varepsilon^2_{n,d}]^T, \hspace{1cm} \varepsilon^3 \triangleq [\varepsilon^3_{1,1}, \ldots, \varepsilon^3_{n,d}]^T.
\]

Substituting (28) in (29) we have:

\[
\Delta \triangleq \psi(B_1^T, b_2^2) - \psi(b_1^1, b_2^2) - \kappa^T \varepsilon^1 - \kappa^2 \varepsilon^2 - \kappa^3 \varepsilon^3
\]

\[
\leq \frac{1}{T} \left( \frac{\rho}{2} \|Bb^2\|^2 + \frac{1}{2\rho} \|\kappa^1\|^2 + \frac{1}{2\rho} \|\kappa^2\|^2 + \frac{1}{2\rho} \|\kappa^3\|^2 \right).
\]  \hspace{1cm} \text{(29)}
Proof. Add up both sides of Lemma 7 and Lemma 6 and subtract $\psi(b^*_1, b^*_2)$. The total approximation error due to ADMM optimization schema is $LHS$:

$$LHS \triangleq \frac{1}{n} \sum_i (\tilde{f}_T(x_i) - y_i)^2 + \lambda \|f\| - \min_f \left( \frac{1}{n} \sum_i (\tilde{f}(x_i) - y_i)^2 + \lambda \|f\| \right)$$

$$\leq \psi(\hat{b}_T^1, \hat{b}_T^2) - \psi(b^*_1, b^*_2)$$

$$+ \frac{1}{n} \sum_i (\varepsilon_{i,i}^1)^2 + 2 \sqrt{\frac{1}{n} \sum_i (\max_j \varepsilon_{i,j}^1)^2} \left( 1 + \frac{1}{T} \sqrt{n \lambda^2} \right) + \lambda \sum_i (\max_j \varepsilon_{i,j}^2 + \max_i \varepsilon_{i,i}^3)$$

$$\triangleq RHS.$$

Assume $\varepsilon_1 \leq \varepsilon_2$ then,

$$RHS \leq \psi(\hat{b}_T^1, \hat{b}_T^2) - \psi(b^*_1, b^*_2) + 3 \sqrt{\frac{1}{n} \sum_i (\max_j \varepsilon_{i,j}^1)^2} \left( 1 + \frac{1}{T} \sqrt{n \lambda^2} \right) + \lambda \sum_i (\max_j \varepsilon_{i,j}^2 + \max_i \varepsilon_{i,i}^3).$$

In Eq. (29) set

$$\kappa_{i,j}^1 = \begin{cases} -\frac{3\sqrt{1 + \frac{3\rho n^2}{T \lambda^2}} \varepsilon_{i,j}^1}{\sqrt{n \sum_i (\max_k \varepsilon_{i,k}^1)^2}} & \text{if } j = \arg \max_k \varepsilon_{i,k}^1 \\ 0 & \text{otherwise} \end{cases}$$

$$\kappa_{i,l}^2 = \begin{cases} -\lambda \sign \varepsilon_{i,l}^2 & \text{if } i = \arg \max_k |\varepsilon_{i,k}^2| \\ 0 & \text{otherwise} \end{cases}$$

$$\kappa_{i,l}^3 = \begin{cases} -\lambda \sign \varepsilon_{i,l}^3 & \text{if } i = \arg \max_k |\varepsilon_{i,k}^3| \\ 0 & \text{otherwise} \end{cases}$$

We have

$$RHS = \Delta \leq \frac{1}{T} \left( \frac{\rho}{2} \|Bb^*_2\|^2 + \frac{9}{2n\rho} (1 + \frac{1}{T} \sqrt{n \lambda^2}) + \frac{d}{\rho^2} \lambda^2 \right)$$

$$\leq \frac{1}{T} \left( \frac{9\rho n^2}{T \lambda^2} + \frac{9}{2n\rho} (1 + \frac{1}{T} \sqrt{n \lambda^2}) + \frac{d}{\rho^2} \lambda^2 \right).$$

Set $\rho = \frac{\sqrt{2} \lambda^2}{n}$, and then we get: $LHS \leq RHS = \Delta \leq \frac{6n\sqrt{2}}{T}$ if $\lambda \geq \frac{3}{\sqrt{2nd}}$ and $n\rho T \geq \frac{9}{2}$.

Now assume $\varepsilon_1 \geq \varepsilon_2$. We get:

$$RHS \leq \psi(\hat{b}_T^1, \hat{b}_T^2) - \psi(b^*_1, b^*_2) + 3 \frac{1}{n} \sum_i (\max_j \varepsilon_{i,j}^1)^2 + \lambda \sum_i (\max_j \varepsilon_{i,j}^2 + \max_i \varepsilon_{i,i}^3).$$
We’ll have
\[
\Delta = \psi(\tilde{b}_T^1, \tilde{b}_T^2) - \psi(b_1^*, b_2^*) + 4 \frac{1}{n} \sum_i (\max_j \varepsilon_{i,j}^1)^2 + \lambda \sum_i (\max_i |\varepsilon_{i,l}^2| + \max_i |\varepsilon_{i,l}^3|)
\]
\[
\leq \frac{1}{T} \left( 9 \rho n^2 \frac{\lambda^2}{\lambda^2} + 16 \frac{2 \rho n^2}{\lambda^2} \sum_i (\max_j \varepsilon_{i,j}^1)^2 + \frac{d \rho \lambda^2}{\rho^2} \right)
\]
It’s straightforward to see if \( n \rho T \geq 8 \) we have
\[
LHS \leq RHS \leq \Delta - \frac{16}{2 \rho n^2 T} \sum_i (\max_j \varepsilon_{i,j}^1)^2 = O\left( \frac{1}{T} \left( \frac{\rho n^2}{\lambda^2} + \frac{d \rho \lambda^2}{\rho^2} \right) \right)
\]
Set \( \rho = \frac{\sqrt{d \lambda^2}}{n} \) we get: \( LHS \leq \frac{3 n \sqrt{d}}{T} \). Only if \( T \geq \frac{8}{\sqrt{d \lambda^2}} \). \( \square \)
B Experimental results

This section provides the regression and classification experiment results in tabular format.

Table 1: Comparison of Regression performance on UCI datasets.

| dataset                          | n   | d  | dc | regression | $R^2 \times 100$ |
|----------------------------------|-----|----|----|------------|------------------|
| Parkinson Speech Dataset         | 702 | 52 | -3.7| -4         | -14.8            |
| Garment Productivity             | 905 | 37 | 25.5| 15.2       | 45.9             |
| Concrete Compressive Strength    | 1030| 8  | 91.7| 59.9       | 91.8             |
| Geographical Original of Music-1 | 1059| 68 | 21.9| 16.6       | 25.1             |
| Geographical Original of Music-2 | 1059| 68 | 32.6| 23.8       | 31.3             |
| Solar Flare-1                    | 1066| 23 | 3.3 | 6.1        | -28              |
| Solar Flare-2                    | 1066| 23 | -6.1| -2.1       | -17              |
| Airfoil Self-Noise               | 1503| 5  | 95.2| 51.1       | 93.3             |
| Communities and Crime            | 1994| 122| 62.1| 64.5       | 65.4             |
| SML2010                          | 3000| 24 | 90.8| 96         | 93.4             |
| SML2010                          | 3000| 24 | 77.3| 94         | 92.4             |
| Parkinson’s Telemonitoring       | 4406| 25 | 93.8| 98.4       | 92.3             |
| Parkinson’s Telemonitoring       | 4406| 25 | 95.5| 98.5       | 92               |
| Wine Quality                     | 4898| 11 | 51.8| 27.2       | 52.6             |
| Bias Correction of Temperature Forecast-1 | 6200| 52 | 62.9| 60.8       | 64.2             |
| Bias Correction of Temperature Forecast-2 | 6200| 52 | 75.2| 76.5       | 76.3             |
| Seoul Bike Sharing Demand        | 6570| 19 | 89.7| 80.7       | 93.1             |
| Air Quality-1                    | 7110| 21 | 87  | 89.5       | 88.2             |
| Air Quality-2                    | 7110| 21 | 100 | 94.7       | 99.8             |
| Air Quality-3                    | 7110| 21 | 86.6| 86.4       | 87.7             |
| Air Quality-4                    | 7110| 21 | 81.7| 84         | 78.1             |
| Combined Cycle Power Plant       | 9568| 4  | 95.5| 92.9       | 96.5             |

Table 2: Comparison of Classification performance on UCI datasets.

| dataset                          | n   | d  | pbdl | pbdl0 | rand forest | xgboost | pbdl | pbdl0 |
|----------------------------------|-----|----|------|-------|-------------|---------|------|-------|
| Iris                             | 149 | 4  | 96.0 | 98.7  | 96          | 96.6    | 22.1 | 46.2  |
| Wine                             | 178 | 13 | 96.0 | 96.6  | 96.7        | 95.5    | 23.6 | 496.2 |
| Blood Transfusion                | 748 | 4  | 72.6 | 74.8  | 72.9        | 78.4    | 46.3 | 21514.0 |
| Breast Cancer Wisconsin          | 569 | 30 | 94.4 | 96.5  | 96.1        | 96.0    | 114.0| 224407 |
| Balance Scale                    | 625 | 4  | 84.6 | 93.0  | 83          | 92.2    | 150.3| 617.0 |
| Abalone                          | 4177| 10 | 22.6 | N/A   | 24.9        | 26.2    | 3688.0| N/A   |