A Better Computational Framework for L₂E Regression

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Abstract

Building on previous research of [Chi and Chi (2022)], the current paper revisits estimation in robust structured regression under the L₂E criterion. We adopt the majorization-minimization (MM) principle to design a new algorithm for updating the vector of regression coefficients. Our sharp majorization achieves faster convergence than the previous alternating projected gradient descent algorithm (Chi and Chi, 2022). In addition, we reparameterize the model by substituting precision for scale and estimate precision via a modified Newton’s method. This simplifies and accelerates overall estimation. Finally, we introduce distance to set penalties to allow constrained estimation under nonconvex constraint sets. This tactic also improves performance in coefficient estimation and structure recovery. We demonstrate the merits of the refined framework through a rich set of simulation examples.

Keywords: Integral squared error criterion; MM principle; Newton’s method; penalized estimation; distance penalization

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1 Introduction

Linear least squares regression quantifies the relationship between a response and a set of predictors. As such, it has been the most popular and productive technique of classical statistics. The growing complexity of modern datasets necessitates special structures on the vector of regression coefficients. A typical example is sparse regression for high-dimensional data, where the number of predictors exceeds the number of responses. In this setting, assuming the coefficient vector is sparse not only improves a regression model’s interpretability but also improves its prediction accuracy. The most popular vehicle for dealing with sparse regression is the least absolute shrinkage and selection operator (Lasso) (Tibshirani 1996). Other examples of structured regression include isotonic regression (Barlow and Brunk 1972), convex regression (Seijo and Sen 2011), and ridge regression (Hoerl and Kennard 1970).

Unfortunately, least squares estimates are extremely sensitive to outliers. A single outlier can ruin estimation accuracy. Consequently, robust structured regression has gained considerable traction in recent years. Numerous authors have contributed to the current body of techniques. To mention a few, Alvarez and Yohai (2012) propose a family of robust estimates for isotonic regression that replaces the least squares criterion with the M-estimation criterion (Huber 1992). Blanchet et al. (2019) employ absolute error loss in robust convex regression. This is also an instance of an M-estimator. Nguyen and Tran (2012) suggest an extended Lasso method incorporating a stochastic noise term to account for corrupted observations in robust sparse multiple regression. Alfons et al. (2013) add a Lasso penalty to the least trimmed squares (LTS) loss to produce a robust sparse estimator.
that trims outliers by effectively minimizing the sum of squared residuals over a selected subset. Lozano et al. (2016) adopt the minimum distance criterion to design a log-scaled loss function and propose the minimum distance Lasso method for robust sparse regression. Other robust sparse regression methods can be found in (Wang et al., 2007; She and Owen, 2011; Wang et al., 2013).

The above works investigate robust structured regression on a case-by-case basis. Yang et al. (2018) develop a family of trimmed regularized M-estimators with a wider focus but with the need to select the degree of trimming. Recently, Chi and Chi (2022) derive yet another general framework for robust structured regression that simultaneously estimates regression coefficients as well as a precision parameter, which plays the same role as the trimming parameter in Yang et al. (2018). Chi and Chi (2022) use the $L_2E$ criterion (Scott, 1992) to quantify goodness-of-fit and a continuous convex penalty to enforce structure. Their algorithmic framework solves the corresponding optimization problem by block descent. Although the computational framework presented in (Chi and Chi, 2022) is general, there is room for some nontrivial improvements. First, the proposed projected gradient algorithm for updating both the regression coefficients and the precision parameter at each block descent iteration can be slow to converge. Second, the box constraint on the precision parameter introduces two additional hyper-parameters that must be specified. Finally, the limitation of convex constraints excludes important nonconvex constraints that impose desirable structures.

The limitations in (Chi and Chi, 2022) just discussed motivate the current paper and its new contributions. First, we derive a majorization-minimization algorithm to accelerate
the estimation of the regression coefficients. Second, we reparameterize the precision parameter to eliminate the box constraint. A simple one-dimensional approximate Newton’s method quickly solves the resulting smooth unconstrained problem for updating precision. Finally, we demonstrate improved statistical performance by imposing nonconvex penalties. Specifically, we adopt distance-to-set penalties to improve estimation accuracy subject to structural constraints. These improvements do not compromise robustness.

The rest of this paper is organized as follows. In Section 2, we review the $L_2$E criterion, the MM principle, and distance penalization. In Section 3, we set up the optimization problem for robust structured regression under the $L_2$E criterion. In Section 4, we introduce strategies that improve the estimation techniques of (Chi and Chi, 2022). In Section 5, we provide a rich set of examples of structured regression to demonstrate the empirical performance of our new algorithms. We end with a discussion in Section 6.

2 Background

2.1 The $L_2$E Criterion

Although traditionally used in nonparametric estimation, the $L_2$E criterion, also known as the integrated squared error (ISE), can be exploited in parametric settings for robust estimation. Suppose the goal is to estimate a density function $f(x \mid \theta)$, where the true parameter $\theta$, is unknown. The $L_2$E criterion seeks to estimate $\theta$ by minimizing the $L_2$
distance between \( f(x \mid \theta) \) and \( f(x \mid \theta^*) \); thus

\[
\hat{\theta} = \arg\min_{\theta} \int [f(x \mid \theta) - f(x \mid \theta^*)]^2 \, dx
\]  

\[
= \arg\min_{\theta} \int f(x \mid \theta)^2 \, dx - 2 \int f(x \mid \theta) f(x \mid \theta^*) \, dx + \int f(x \mid \theta^*)^2 \, dx. \quad (1)
\]

The third integral in formula (1) does not depend on \( \theta \) and can be excluded from the minimization. The second integral is the expectation of \( f(x \mid \theta) \) and can be approximated by an unbiased estimate, namely its sample mean. Therefore, an approximate \( L_2 \) estimate of \( \theta \) is

\[
\hat{\theta}_{L_2E} = \arg\min_{\theta} \int f(x \mid \theta)^2 \, dx - \frac{2}{n} \sum_{i=1}^{n} f(x_i \mid \theta), \quad (2)
\]

where \( n \) denotes the sample size. The \( L_2E \) estimate represents a trade-off between efficiency and robustness. It is less efficient but more robust than the maximum likelihood estimate (MLE) [Scott 2001; Warwick and Jones 2005]. Chi and Chi (2022) discuss in detail how the \( L_2E \) estimator imparts robustness in structured regression.

### 2.2 The MM Principle

The majorization-minimization (MM) principle [Lange et al. 2000; Lange 2016] for minimizing an objective function \( h(\theta) \) involves two steps, a) majorization of \( h(\theta) \) by a surrogate function \( g(\theta \mid \theta_k) \) anchored at the current iterate \( \theta_k \) and then b) minimization of \( \theta \mapsto g(\theta \mid \theta_k) \) to construct \( \theta_{k+1} \). The surrogate function \( g(\theta \mid \theta_k) \) must satisfy the two requirements:

\[
h(\theta_k) = g(\theta_k \mid \theta_k), \quad \text{tangency} \quad (3)
\]

\[
h(\theta) \leq g(\theta \mid \theta_k) \quad \forall \theta, \quad \text{domination}. \quad (4)
\]
Under these conditions, the iterates enjoy the descent property \( h(\theta_{k+1}) \leq h(\theta_k) \) as demonstrated by the relations

\[
h(\theta_{k+1}) \leq g(\theta_{k+1} | \theta_k) \leq g(\theta_k | \theta_k) = h(\theta_k),
\]
reflecting conditions (3) and (4). Ideally, the MM principle converts a hard optimization problem into a sequence of easier ones. The key to success is the construction of a tight majorization that can be easily minimized. In practice, majorization can be done piecemeal by exploiting the convexity or concavity of the various terms comprising the objective.

### 2.3 Distance Penalization

To estimate a parameter vector \( \theta \) subject to a set constraint \( \theta \in C \), it is often convenient to employ a squared Euclidean distance penalty (Chi et al., 2014; Xu et al., 2017). For a closed set \( C \), the penalty is defined as

\[
\frac{1}{2} \text{dist}(\theta, C)^2 = \min_{\beta \in C} \frac{1}{2} \|\theta - \beta\|_2^2.
\]

(5)

The beauty of this penalty is that it is majorized at the current iterate \( \theta_k \) by the spherical quadratic

\[
\frac{1}{2} \|\theta - \mathcal{P}_C(\theta_k)\|_2^2.
\]

(6)

where \( \mathcal{P}_C(\theta) \) denotes the Euclidean projection of \( \theta \) onto \( C \) (Bauschke and Combettes, 2011). When \( C \) is both closed and convex, \( \mathcal{P}_C(\theta) \) consists of a single point. For nonconvex sets, \( \mathcal{P}_C(\theta) \) sometimes consists of multiple points. When \( \mathcal{P}_C(\theta) \) is single valued, the distance penalty (5) has gradient \( \theta - \mathcal{P}_C(\theta) \)
The proximal distance method of constrained optimization minimizes the penalized objective \( h(\theta) + \frac{\rho}{2} \text{dist}(\theta, C)^2 \) \( \text{[Xu et al., 2017; Keys et al., 2019]} \). The tuning constant \( \rho \) controls the trade-off between minimizing the loss \( h(\theta) \) and satisfying the constraint \( \theta \in C \). In practice, a large \( \rho \) is chosen to enforce the constraint. The MM principle suggests majorizing the distance penalty by the spherical quadratic \( [\theta] \) and applying the proximal map \( \theta_{k+1} = \text{prox}_{\rho^{-1}h}[\mathcal{P}_C(\theta_k)] \) to generate the next iterate. The proximal distance principle applies to a wide array of models, including sparse regression, nonnegative regression, and low-rank matrix completion. It is accurate in estimation and avoids the severe shrinkage of Lasso penalization \( \text{[Xu et al., 2017; Landeros et al., 2020]} \) extend distance penalization to fusion constraints of the form \( D\beta \in C \) involving a fusion matrix \( D \) such as a discrete difference operator. Although the advantages of proximal maps are lost, this extension brings more constrained statistical models under the umbrella of distance penalization.

3 L₂E Robust Structured Regression

Consider the classical linear regression model \( y = X\beta + \tau^{-1} \epsilon \), where \( y \in \mathbb{R}^n \) is the response vector, \( X \in \mathbb{R}^{n \times p} \) is the design matrix of predictors, and \( \epsilon \in \mathbb{R}^n \) is the noise vector with independent standard Gaussian components. The regression coefficients \( \beta \in \mathbb{R}^p \) and the precision \( \tau \in \mathbb{R}_+ \) are the parameters of the model. Collectively, we denote the parameters by \( \theta = (\beta^T, \tau)^T \). The density of the \( i \)th response \( y_i \) amounts to

\[
f(y_i \mid \theta) = \frac{\tau}{\sqrt{2\pi}} e^{-\frac{\epsilon_i^2}{2\tau}},
\]
where \( r_i = y_i - x_i^T \beta \) is the \( i \)th residual. A brief calculation shows that equation (2) gives rise to the L\(_2\)E loss

\[
h(\theta) = \int f(y \mid \theta)^2 \, dy - \frac{2}{n} \sum_{i=1}^{n} f(y_i \mid \theta) = \frac{\tau}{2\sqrt{\pi}} - \frac{\tau}{n} \sqrt{\frac{2}{\pi}} \sum_{i=1}^{n} e^{-\frac{r_i^2}{\tau^2}}. \tag{7}
\]

Structured regression introduces set constraints on the regression coefficient vector \( \beta \). Consequently, L\(_2\)E aims to solve the constrained optimization problem

\[
\min_{\beta \in \mathbb{R}^p, \tau \in \mathbb{R}^+} h(\beta, \tau), \quad \text{subject to} \quad \beta \in C. \tag{8}
\]

For example, \( C = \{ \beta \in \mathbb{R}^p : \beta_1 \leq \beta_2 \leq \cdots \leq \beta_p \} \) leads to a robust isotonic regression problem. Sparsity can be imposed directly by taking \( C = \{ \beta \in \mathbb{R}^p : \|\beta\|_0 \leq k \} \) for some positive integer \( k \) or indirectly by taking \( C = \{ \beta \in \mathbb{R}^p : \|\beta\|_1 \leq t \} \) for \( t > 0 \). Alternatively, we can rewrite problem (8) as the non-smooth optimization problem

\[
\min_{\beta \in \mathbb{R}^p, \tau \in \mathbb{R}^+} [h(\beta, \tau) + \phi(\beta)], \tag{9}
\]

where the penalty \( \phi(\beta) \) is either the \( 0/\infty \) indicator of the constraint set \( C \) denoted by \( \iota_C(\beta) \) or a better behaved but still non-smooth substitute such as the Lasso.

Solving problem (8), or equivalently solving (9), is challenging for two reasons. First, both problems are nonconvex owing to the nonconvexity of the L\(_2\)E loss (7). Second, the penalty term \( \phi(\beta) \) may be non-differentiable. Fortunately, the block gradients of the L\(_2\)E loss with respect to \( \beta \) and \( \tau \), \( \nabla_\beta h(\beta, \tau) \) and \( \frac{\partial}{\partial \tau} h(\beta, \tau) \), are Lipschitz. This key property motivates a block descent algorithm in [Chi and Chi, 2022] that alternates between reducing the objective with respect to \( \beta \) and \( \tau \), holding the other block fixed. [Chi and Chi, 2022] also impose the bounds \( 0 < \tau_{\min} \leq \tau \leq \tau_{\max} < \infty \) on \( \tau \).
An appealing property of block descent is that the objective function is guaranteed to decrease at each iteration. [Chi and Chi (2022)] apply projected gradient descent to decrease the objective in each block update. Because the projected gradient updates are based on a loose loss majorization, the algorithm is slow to converge. To ameliorate this fault, we propose new strategies for updating $\beta$ and $\tau$ in the next section.

## 4 Computational Methods

### 4.1 Updating the Regression Coefficients

Consider the problem of updating the regression coefficients $\beta$. Because the contribution $-e^{-\tau^2 r_i^2 / 2}$ to the L$_2$E loss (7) is differentiable and concave with respect to $r_i^2$, we can exploit the concave majorization

\[
f(u) \leq f(u_k) + f'(u_k)(u - u_k)
\]

in the form

\[
-e^{-\tau^2 r_i^2 / 2} \leq -e^{-\tau^2 r_{ki}^2 / 2} + \frac{\tau^2}{2} e^{-\tau^2 r_{ki}^2 / 2} (r_i^2 - r_{ki}^2)
\]

around the tangency point $r_{ki}^2$. By omitting irrelevant multiplicative and additive terms, this produces the surrogate function

\[
f(\beta | \beta_k, \tau) = \frac{1}{2} \sum_{i=1}^{n} e^{-\tau^2 r_{ki}^2 / 2} (y_i - x_i^T \beta_k)^2 = \frac{1}{2} \| \tilde{y} - \tilde{X}\beta \|_2^2
\]

for the L$_2$E loss (7), where $r_{ki} = y_i - x_i^T \beta_k$ is the $i$th residual at iteration $k$, $\tilde{y} = \sqrt{W_k} y$, $\tilde{X} = \sqrt{W_k} X$, and $W_k \in \mathbb{R}^{n \times n}$ is a diagonal matrix with $i$th diagonal entry $e^{-\tau^2 r_{ki}^2 / 2}$. 
The next proposition demonstrates that the surrogate \((11)\) is the sharpest quadratic majorization in the residual variables \(r_i\). A sharp majorization hugs the objective function tightly and accelerates the convergence of the corresponding MM algorithm \(\text{[de Leeuw and Lange, 2009]}\). The proposition does not claim that the majorization \((11)\) is the sharpest multivariate quadratic majorization in the full variable \(\beta\). Despite this fact, the majorization yields substantial gains in computational efficiency over the looser projected gradient majorization pursued by \(\text{[Chi and Chi, 2022]}\).

**Proposition 4.1.** Let \(f(r) = -e^{-ar^2}\) with \(a > 0\). Then the symmetric quadratic function \(g(r) = -e^{-ar^2} + ae^{-ar^2}(r^2 - r_k^2)\) is a sharp quadratic majorizer of \(f(r)\).

**Proof.** \(\text{[van Ruitenburg, 2005]}\) proves that a univariate quadratic function \(g(r)\) majorizing a univariate differentiable function \(f(r)\) and touching it at two points is sharp. In the present case, \(g(r)\) touches \(f(r)\) at the points \(r = \pm r_k\).

For an \(L_2E\) loss with penalty \(\phi(\beta)\), the next MM iterate is

\[
\beta_{k+1} = \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2} \left\| \tilde{y} - \tilde{X}\beta \right\|^2_2 + \phi(\beta).
\]

In the setting of distance penalization with a fusion penalty, the surrogate reduces to the least squares criterion

\[
\frac{1}{2} \left\| \begin{pmatrix} \tilde{y} \\ \sqrt{\rho}P_C(D\beta_k) \end{pmatrix} - \begin{pmatrix} \tilde{X} \\ \sqrt{\rho}D \end{pmatrix}\beta \right\|^2_2,
\]

which is amenable to minimization by the QR algorithm or the conjugate gradient algorithm. The computational complexity of the \(\beta\) update is dominated by this least squares problem. Indeed, computation of the current residuals, the matrix \(W_k\), the product \(\tilde{y}\), and
the product $\tilde{X}$ require, respectively, operation counts of $O(np)$, $O(n)$, $O(n)$, and $O(np)$. Updating $\beta$ using projected gradient descent requires similar steps. Evaluation of the proximal map of $\phi(\beta)$ reduces to penalized least squares with an identity design matrix. Hence, the computational cost per iteration of the current MM algorithm is essentially the same as that of the projected gradient descent algorithm in [Chi and Chi 2022]. The numbers of iterations until convergence of the two algorithms are vastly different however. Additionally, the distance penalized MM algorithm is more flexible in allowing nonconvex and fusion constraints.

4.2 Updating the Precision Parameter

There are two concerns in updating $\tau$, namely the slow convergence of projected gradient descent and the presence of box constraints on $\tau$. To attack the latter concern, we reparameterize by setting $\tau = e^\eta$ for $\eta$ real. Because the stationary condition for minimizing the loss $h(\beta, e^\eta)$ with respect to $\eta$ is intractable, we turn to a variant of Newton’s method. The required first and second derivatives are

$$\frac{\partial}{\partial \eta} h(\beta, e^\eta) = \frac{e^n}{2\sqrt{\pi}} - \frac{e^n}{n} \sqrt{\frac{2}{\pi}} \sum_{i=1}^{n} w_i + \frac{e^{3n}}{n} \sqrt{\frac{2}{\pi}} \sum_{i=1}^{n} w_i r_i^2$$

$$\frac{\partial^2}{\partial \eta^2} h(\beta, e^\eta) = \frac{e^n}{2\sqrt{\pi}} + \frac{4e^{3n}}{n} \sqrt{\frac{2}{\pi}} \sum_{i=1}^{n} w_i r_i^2 - \frac{e^n}{n} \sqrt{\frac{2}{\pi}} \sum_{i=1}^{n} w_i - \frac{e^{5n}}{n} \sqrt{\frac{2}{\pi}} \sum_{i=1}^{n} w_i r_i^4,$$

where $w_i = e^{-e^{2n}r_i^2/2}$ and $r_i$ is the $i$th residual. The Newton increment only points downhill when $\frac{\partial^2}{\partial \eta^2} h(\beta, e^\eta)$ is positive. This prompts discarding the negative contributions and relying on the approximation

$$\frac{\partial^2}{\partial \eta^2} h(\beta, e^\eta) \approx d = \frac{e^n}{2\sqrt{\pi}} + \frac{4e^{3n}}{n} \sqrt{\frac{2}{\pi}} \sum_{i=1}^{n} w_i r_i^2.$$
Our modified Newton’s iterates are defined by

\[ \eta_{k+1} = \eta_k - t_k d_k^{-1} \frac{\partial}{\partial \eta} h(\beta, e^{\eta_k}), \]

where \( t_k \) is a positive stepsize parameter chosen via Armijo backtracking started at \( t_k = 1 \). Little backtracking is needed because replacing \( \frac{\partial^2}{\partial \eta^2} h(\beta, e^{\eta}) \) by the larger value \( d \) diminishes the chances of overshooting the minimum of \( h(\beta, e^{\eta}) \).

Our modified Newton’s method enjoys the same computational complexity as projected gradient descent. The dominant computational expense in updating \( \eta \) in both algorithms comes from computing the residuals \( r_i \). This step requires \( O(np) \) operations. Once all \( r_i \) are updated, computing the derivatives only requires an additional \( O(n) \) operations. In summary, our new strategy converges in fewer iterations, removes the box constraint on \( \tau \), and enjoys the same computational cost per iteration as projected gradient descent.

Algorithm 1 summarizes our algorithm for minimizing the penalized loss (9). As in (Chi and Chi, 2022), we update \( \beta \) and \( \eta \) \( N_\beta \) and \( N_\eta \) times, respectively, in each block descent iteration. Note that we use \( W_+ \) to denote its dependence on the previous iterate \( \beta_+ \).

## 5 Numerical Experiments

To compare the computational efficiency of Algorithm 1 (abbreviated MM) and projected gradient descent (abbreviated PG), we consider isotonic regression and convex regression. To highlight the advantages of distance penalization over leading penalization methods, we consider sparse regression and trend filtering.
Algorithm 1 Block descent with MM and approximate Newton for problem (9)

Initialize: $\beta_0 \in \mathbb{R}^p$, $\tau_0 \in \mathbb{R}_+$, $N_\beta$, and $N_\eta$.

1: for $k = 1, 2, \cdots$ do
2: \hspace{1em} $\beta^+ \leftarrow \beta_{k-1}$
3: \hspace{1em} for $i = 1, \cdots, N_\beta$ do
4: \hspace{2em} $\tilde{y} = \sqrt{W_y} y$
5: \hspace{2em} $\tilde{X} = \sqrt{W_x} X$
6: \hspace{2em} $\beta^+ = \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2} \| \tilde{y} - \tilde{X} \beta \|^2_2 + \phi(\beta)$
7: \hspace{1em} end for
8: \hspace{1em} $\beta_k \leftarrow \beta^+$
9: \hspace{1em} $\eta^+ \leftarrow \log(\tau_{k-1})$
10: \hspace{1em} for $i = 1, \cdots, N_\eta$ do
11: \hspace{2em} $\eta^+ = \eta^+ - t_i d_i^{-1} \frac{\partial}{\partial \eta} h(\beta_k, e^{\eta^+})$
12: \hspace{1em} end for
13: \hspace{1em} $\tau_k \leftarrow e^{\eta^+}$
14: end for

5.1 Robust Isotonic Regression

Classical isotonic regression involves minimizing the least squares criterion

$$\| y - \beta \|^2_2 = \sum_{i=1}^n (y_i - \beta_i)^2$$

subject to $\beta$ belonging to the set $C_1 = \{ \beta \in \mathbb{R}^n : \beta_1 \leq \cdots \leq \beta_n \}$. Independent standard normal errors are implicit in this formulation. Here the design matrix $X = I_n$, and the mean function of the model is monotonically increasing and piecewise constant. In the L$_2$E version of the problem, we impose the 0/\infty penalty $\phi(\beta) = \iota_{C_1}(\beta)$. The MM update of $\beta$ succumbs to the \texttt{gpava} function in the \texttt{isotone} R package \cite{deLeeuw2010}. As mentioned earlier, the MM $\beta$ update enjoys the same per-iteration computational cost as the PG $\beta$ update \cite{Chi2022}.

In our simulation, 1000 responses are generated by sampling points $x_i$ evenly from $[-2.5, 2.5]$ and setting $y_i = x_i^3 + s_i + \epsilon_i$, where the $\epsilon_i$ are i.i.d. standard normal deviates, and the $s_i$ shift the underlying cubic signal. The responses define mean vector $\beta \in \mathbb{R}^{1000}$. 

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Outliers are introduced at consecutive responses from the first quartile of the $x_i$ on by setting $s_i = 14$; all other responses have $s_i = 0$. Each method is tested over 100 replicates.

Figure 1 displays boxplots of the MSEs and run times in seconds in fitting the isotonic regression model. We include the results from ordinary least squares (abbreviated LS) as a baseline. As anticipated, the estimation error of LS degrades as the number of outliers increases. In contrast, both MM and PG exhibit much more modest increases in estimation error, with MM less sensitive to outliers than PG. On the other hand, the right panel of Figure 1 shows the significant speed advantage of MM over PG. The run times of PG increase rapidly as the number of outliers increases, while the run times of MM are far more stable and only slightly larger than those of LS. Thus, MM under the $L_2E$ loss retains the speed advantages of LS while mitigating its sensitivity to outliers.

The difference in run time between the PG and MM algorithms is directly attributable to the reduced number of outer iterations until convergence. For the same experiments, Figure 2 depicts boxplots of the mean number of outer block descent iterations, the mean number of inner iterations for updating $\beta$ per outer iteration, and the mean number of
Figure 2: Boxplots of the mean number of outer block descent iterations (left panel), the mean number of inner iterations for updating $\beta$ per outer iteration (middle panel), and the mean number of inner iterations for updating $\tau$ per outer iteration (right panel). All plots refer to the experiments summarized in Figure 1.

It may seem paradoxical that PG takes fewer inner iterations than MM to update $\beta$. However, recall that PG is fitting a less snug surrogate than MM. PG also takes far more inner iterations than MM to update $\tau$. This reflects the speed of our approximate Newton method.

5.2 Robust Convex Regression

Although convex regression and isotonic regression share the same squared loss, their constraint sets differ. Convex regression imposes the constraints $\beta_{i+1} \leq \frac{1}{2}(\beta_i + \beta_{i+1})$ for $1 \leq i < n - 1$ and equally spaced points $x_i$. Collectively, these constraints can be expressed as the constraint set $C_2 = \{\beta \in \mathbb{R}^n : D\beta \geq 0\}$, where $D$ is the corresponding second-order difference matrix. In the $L_2E$ version of the problem, we apply the $0/\infty$ penalty.
Figure 3: Simulation for convex regression. Boxplots depict the MSE (left panel) and running time (right panel) for over 100 replicates under different number of outliers.

\[ \phi(\beta) = \iota_C(\beta) \]. The MM update of \( \beta \) can be computed by the \texttt{conreg} function in the \texttt{cobs} R package \cite{NgMaechler2007}. The MM \( \beta \) update for convex regression again requires the same computational cost as the PG \( \beta \) update \cite{ChiChi2022}.

In our numerical experiment, the components of the mean vector \( \beta \in \mathbb{R}^{500} \) conforms to the quartic function \( x_i^4 + x_i \). Two kinds of perturbations are added to generate the responses \( y_i = x_i^4 + x_i + s_i + \varepsilon_i \). Here the \( x_i \) are sampled evenly from \([-2, 2]\), the \( s_i \) shift the underlying quartic signal, and the \( \varepsilon_i \) are i.i.d. standard normal deviates. Outliers are introduced at consecutive responses from the first quartile of \( x_i \) onward by setting the corresponding shifts \( s_i = 14 \); for all other responses \( s_i = 0 \).

Figure 3 presents boxplots of the MSEs and run times in seconds in fitting the convex regression model with 100 replicates. The estimation accuracy of LS and PG degrades as the number of outliers increases, while MM behaves stably with outliers. As the right panel of Figure 3 shows, the run times of PG quickly increase as the number of outliers increases, while the run times of MM are relatively immune to outliers and comparable.
Figure 4: Boxplots of the mean number of outer block descent iterations (left panel), the mean number of inner iterations for updating \( \beta \) per outer iteration (middle panel), and the mean number of inner iterations for updating \( \tau \) per outer iteration (right panel). All plots refer to the experiments summarized in Figure 3 to those of LS. Thus, MM under the \( L_2E \) loss enjoys the speed advantages of LS while protecting against outliers. To fully comprehend the difference in run times between PG and MM, Figure 4 displays boxplots of the mean number of outer block descent iterations, the mean number of inner iterations for updating \( \beta \) per outer iteration, and the mean number of inner iterations for updating \( \tau \) per outer iteration. MM takes not only fewer outer iterations than PG but also fewer average inner iterations to update \( \beta \) and \( \tau \). This contributes to the distinct speed advantage of MM over PG on convex regression.

### 5.3 Robust Sparse Regression

Sparse linear regression minimizes the penalized least squares criterion

\[
\frac{1}{2} \| \mathbf{y} - \mathbf{X}\beta \|_2^2 + \phi(\beta),
\]
with \( \phi(\mathbf{\beta}) \) promoting sparsity. Typical choices of \( \phi(\mathbf{\beta}) \) includes the Lasso and the nonconvex MCP penalty (Zhang et al., 2010). In the L_{2E} framework, each MM update solves a \( \phi \)-penalized least squares problem. The \texttt{ncvfit} function in the R package \texttt{ncvreg} is ideal for this purpose (Breheny and Huang, 2011). In the distance penalty context, the constraint set is \( C_3 = \{ \mathbf{\beta} \in \mathbb{R}^p : \|\mathbf{\beta}\|_0 \leq k \} \), where the the positive integer \( k \) encodes the sparsity level. The MM update of \( \mathbf{\beta} \) relies on the proximal distance principle and reduces to least squares.

To shed light on the statistical performance of L_{2E} regression with Lasso, MCP, and distance penalties, we undertake a small simulation study involving a sparse coefficient vector \( \mathbf{\beta} = (2, 2, 2, 2, 0, \cdots, 0)^T \in \mathbb{R}^{50} \) and a design matrix \( \mathbf{X} \in \mathbb{R}^{200 \times 50} \) whose independent entries are standard Gaussian deviates. The response \( \mathbf{y} \) is simulated as \( \mathbf{y} = \mathbf{X}\mathbf{\beta} + \mathbf{\epsilon} \) where components of \( \mathbf{\epsilon} \) are standard normal noises. We then shift the first \( m \) entries of \( \mathbf{y} \) and the first \( m \) rows of \( \mathbf{X} \) to produce observations that are outlying with respect to the responses and also high leverage with respect to the predictors. The number of outliers \( m \) is chosen from the grid \{10, 20, 30, 50\}. For the distance penalization, the ideal choice of the sparsity parameter \( k \) is 5. We employ five-fold cross-validation to select the tuning parameters for all three penalties. The sparsity level \( k \) for distance penalization is varied over the grid \{3, 4, 5, 6, 7, 8\}, and the penalty constant \( \rho \) is set to \( 10^8 \). All performance metrics depend on 100 replicates. These metrics include: (a) estimation accuracy, measured by the relative error compared to the true \( \mathbf{\beta} \), and (b) support recovery, measured by the F1 score, the number of true positives, and the number of false positives. The F1 score (harmonic mean of precision and recall) accounts for both true and false positives and takes on values in
Figure 5: Simulation results for sparse regression. Median performance based on 100 replicates for each method under different numbers of outliers.

[0, 1], with a higher score indicating better support recovery.

Figure 5 shows the performance of the Lasso, MCP, and distance penalties in robust sparse regression under the $L_2E$ loss. Distance penalization consistently achieves a low relative error, even when a quarter of the data are contaminated and both Lasso and MCP produce unacceptable estimates. When the number of outliers is relatively small, estimation errors obtained by the Lasso and MCP are relatively low, but still higher than those of distance penalization. Distance penalization consistently delivers a much higher F1 score than Lasso and MCP penalization. The two plots in the bottom row of Figure 5 highlight the difference in support recovery for the three methods. All three identify
the five true positives in each simulation scenario, but the Lasso and MCP suffer from a large number of false positives, selecting many irrelevant predictors. By contrast, distance penalization maintains a low false positive rate. This example emphasizes the flexibility of the L2E framework in accommodating different penalizations and the advantages of distance penalization in both estimation accuracy and structure recovery.

5.4 Robust Trend Filtering

Trend filtering and shape constrained regression as exemplified by isotonic and convex regression illustrate the complexities encountered in combining L2E regression with distance penalization, sparsity recovery, and fusion constraints. The simplest version of trend filtering imposes sparsity on the differences $\beta_{i+1} - \beta_i$. The penalty can be expressed as $\phi(\beta) = \|D\beta\|_0$, where $D$ is a difference matrix and $\|\theta\|_0$ counts the number of nonzero entries of $\theta$. Thus, if the underlying trend is piecewise constant, then $D$ is a first-order difference matrix. If the trend is piecewise affine, then $D$ is a second-order difference matrix. In practice, the problem is often convexified by substituting an $\ell_1$ penalty for the $\ell_0$ penalty. With this change, it is possible to treat the MM update of $\beta$ as a generalized lasso problem and use the genlasso function in the R package genlasso (Arnold and Tibshirani, 2019) to compute the solution.

A brief study of trend filtering under the L2E loss and the distance and $\ell_1$ penalties is illuminating. The simulated data consists of four consecutive segments with $\beta$ values $-2, 5, 0,$ and $-10$ and jumps at 50, 100, and 150. The components of $\beta$ are randomly perturbed by standard Gaussian deviates to create the observed responses $y_i$. Random responses
are then shifted by 2 to produce outliers. Distance penalization invokes the constraint set
\[ C_4 = \{\beta \in \mathbb{R}^{200} : \|D\beta\|_0 \leq k\} \]
where \(D\) is the first-order difference matrix and the tuning parameter \(k\) denotes the number of jumps in \(\beta\). Ideally, we should find the sparsity level \(k = 3\). We examine \(k\) over the grid \(\{1, 2, 3, 4, 5, 6\}\) and employ five-fold cross-validation to select \(k\). The penalty constant \(\rho\) is set to \(10^8\). Under the \(\ell_1\) penalty \(\lambda \|D\beta\|_1\), we also choose \(\lambda\) by five-fold cross-validation and declare a jump whenever the magnitude of a component \(D\hat{\beta}\) exceeds 0.01. For both penalties, we measure estimation accuracy by the MSE of the trend estimate \(\hat{\beta}\). Structure recovery is determined by the number of true and false jumps.

Figure 6 summarizes the median performance of the \(\ell_1\) and the distance penalties in robust trend filtering under the \(L_2E\) loss over 50 replicates. As expected, MSE increases as the number of outliers increases. Distance penalization always achieves a lower MSE than \(\ell_1\) penalization. Both methods successfully capture the three true jumps in the trend component, but \(\ell_1\) penalization produces more undesirable false jumps than distance penalization. Figure 7 displays an example of the trend estimates delivered by the two different
penalization methods. Distance penalization recovers the jumps in the trend component more effectively than $\ell_1$ penalization. Furthermore, the smooth segments obtained by distance penalization are closer to the truth than those obtained by $\ell_1$ penalization. This trend filtering example once again shows the flexibility of the L2E framework and the advantages of distance penalization.

6 Discussion

Because robust structured regression is resistant to the undue influence of outliers, it is valuable in many noisy data applications. The L2E computational framework (Chi and Chi, 2022) for robust structured regression has the advantage of allowing the simultaneous estimation of regression coefficients and precision. Nevertheless, the original computational framework has its drawbacks. Its estimation procedure is slow to converge, and its penalties must be convex. This paper attacks both limitations while retaining the overall strategy of block descent. We introduce an MM algorithm based on a sharp majorization to accelerate convergence. Each MM update of $\beta$ reduces to penalized least squares and can be readily handled by existing regression solvers. Although this plug-and-play tactic already formed
part of the projected gradient algorithm in (Chi and Chi, 2022), our tight majorization leads to better results. We also reparameterize precision to avoid box constraint and update the new precision parameter by an approximate Newton’s method. The computational cost per iterate remains the same, but again the number of iterations until convergence drops considerably. Finally, we extend penalization to distance and nonconvex penalties. These steps lead to better statistical performance and model selection.

We demonstrate the merits of our refined computational framework through a rich set of simulation examples, including isotonic regression, convex regression, sparse regression, and trend filtering. Given the same penalties, our simulation results show that the new algorithms outperform the original ones in both computational speed and estimation accuracy. Distance penalties to sparsity sets, in particular, show competitive advantages in both estimation accuracy and model selection. Overall, the innovations introduced here make $L^2E$ an attractive tool for robust structured regression.

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