Sparsity by Worst-Case Quadratic Penalties

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Abstract
This paper proposes a new robust regression interpretation of sparse penalties such as the elastic net and the group-lasso. Beyond providing a new viewpoint on these penalization schemes, our approach results in a unified optimization strategy. Our evaluation experiments demonstrate that this strategy, implemented on the elastic net, is computationally extremely efficient for small to medium size problems. Our accompanying software solves problems at machine precision in the time required to get a rough estimate with competing state-of-the-art algorithms.

Keywords: sparse regression, robust optimization, lasso, elastic net, group-lasso

1. Introduction
Robust optimization aims at solving problems where data is uncertain. This viewpoint has recently been investigated in machine learning, providing novel interpretations of well-known methods, thereby opening new perspectives for their analysis [Ben-Tal et al. 2009].

Support vector machines can be interpreted in the robust optimization framework under the corrupted location model [Caramanis et al. 2012], which assumes that uncertainty affects input variables. More closely related to our present concerns, Lasso has been shown to be the solution of a robust least squares problem where input variables are assumed to be corrupted by a feature-wise disturbance [Xu et al. 2010].

In this paper, we introduce a new robust regression interpretation of sparse penalties, where both the design matrix and the output variable are assumed to be corrupted. We
suppose that responses are affected by an adversarial noise, and according to the properties of this noise, several sparsity-inducing penalties can be recovered. We use this formalism to derive a general-purpose algorithm for solving classical sparse regression problems.

Robust optimization leads to formalizing minimax problems. In our approach, the inner problem is a simple unconstrained quadratic problem, and we propose an optimization strategy based on the iterative resolution of plain quadratic problems. The approach is highly competitive compared to state-of-the-art optimization strategies for sparse regression such as coordinate descent (Fu, 1998) or proximal methods (Beck and Teboulle, 2009). The general-purpose algorithm introduced in this paper relies on second order techniques to solve a series of quadratic approximations to the sparse regression problem. Our solver is thus applicable to small and medium size problems (that is, problems from several hundreds to a few thousands of active variables on a current computer), where it is very accurate and faster than the first order techniques mentioned above.

Section 2 introduces our general robust regression formalization, which allows numerous variants that follow from the definition of the uncertainty set on the adversarial noise, thereby leading to different sparse regression problems. Section 3 fully details the derivations for the Lasso and the group-Lasso (using the $\ell_{\infty,1}$ mixed-norm) problems, applied together with an $\ell_2$ ridge penalty (leading to what is known as the elastic net for the Lasso). A description of the general-purpose active set algorithm derived from this formalism is given in Section 4, which also introduces a new bound on the optimality gap stemming from the new formalization and the resolution scheme. Finally, Section 5 demonstrates that our solver is highly efficient compared to existing algorithms and popular implementations.

2. Robust Optimization Framework

As a simple motivating example, we consider a model where the response variable $Y$ is assumed to be linearly related to the $p$ predictor variables $X = (X_1, \ldots, X_p)$:

$$ Y = X\beta^* + \varepsilon, \quad (1) $$

where $\beta^*$ is the vector of unknown parameters, assumed to be sparse, and $\varepsilon$ is a perturbation variable. We wish to estimate the regression coefficients $\beta^*$ based on training data consisting of an $n \times p$ design matrix $X$ and a response vector $y \in \mathbb{R}^n$. Here, we assume some deviations from the standard linear model, by considering that several sources of uncertainty affect the training data.

Assumption 1 The design matrix $X$ has been corrupted by an unobserved additive perturbation $\Delta X \in D_X$, such that

$$ D_X = \{ \Delta X \in \mathbb{R}^{n \times p} : \|\Delta X\|_F \leq \eta \} \text{ ,} $$

where $\|\cdot\|_F$ is the Frobenius norm. The “true” design matrix corresponding to the $X$ variable of Equation (1) is thus $X - \Delta X$. In addition, the perturbation $\varepsilon$ affects the linear

\footnote{1. This classic uncertainty set of the robust regression literature (Caramanis et al., 2012) may appear in stronger forms ($2$-induced norm for Chandrasekaran et al., 1998), (spectral radius of $\Delta X$ for El Ghaoui and Lebret, 1997). Though defining different sets, these options lead here to the same worst-case solution.}
relationship between the observed $X$ and $y$ via the following decomposition:

$$
\varepsilon = X\gamma + \epsilon,
$$

(2)

where $\gamma$ does not follow the sparsity pattern of $\beta^\star$. The $X\gamma$ component of $\varepsilon$ "adversarially" affects the linear relationship between $X$ and $y$, while $\epsilon$ represents a "neutral" perturbation, which is assumed to belong to the following uncertainty set:

$$
D_\varepsilon = \left\{ \epsilon \in \mathbb{R}^n : \frac{1}{n}\|\epsilon\|_2 \leq \eta_\varepsilon \right\},
$$

(3)

where $\|\cdot\|_2$ is the Euclidean norm (more generally, $\|\cdot\|_p$ will denote the $\ell_p$-norm). These assumptions entail the following relationship between $X$ and $y$:

$$
y = (X - \Delta X)\beta^\star + X\gamma + \epsilon.
$$

That is, the observed responses are formed by summing the contributions of the unobserved clean inputs, the adversarial noise that maps the observed inputs to the responses, and the neutral noise.

We will examine several assumptions about the adverse regression coefficients $\gamma$ that will be discussed in details in Section 3. They state that $\gamma \in D_\gamma$, where $D_\gamma$ is a convex neighborhood of $0$ in $\mathbb{R}^p$, and also that the global uncertainty set on $(\Delta X, \epsilon, \gamma)$ is the Cartesian product $D_X \times D_\epsilon \times D_\gamma$.

Note that we only consider uncertainty sets with finite support, which are amenable to a worst-case analysis. These sets are also relevant for unbounded deviations, in which case they typically represent the confidence regions associated to a prescribed confidence level. In particular, the neutral noise model (3) can be derived as a confidence interval for the centered homoscedastic Gaussian noise that is usually assumed in the linear regression model.

Given the observed training data $(X, y)$, robust estimation considers the problem of minimizing the worst-case scenario, so as to ensure a valid estimation for any perturbation belonging to the uncertainty set. For the time being, even without specifying the form of the uncertainty set $D_\gamma$, one can derive a simple equivalent form of the robust regression problem.

**Proposition 1** The robust regression problem

$$
\min_{\beta \in \mathbb{R}^p} \max_{(\Delta X, \epsilon, \gamma) \in D_X \times D_\epsilon \times D_\gamma} ||(X - \Delta X)\beta + X\gamma + \epsilon - y||_2,
$$

(4)

where $D_X$, $D_\gamma$ and $D_\epsilon$ are defined as in Assumption 1 is equivalent to the robust regularized regression problem:

$$
\min_{\beta \in \mathbb{R}^p} \max_{\gamma \in D_\gamma} ||X\beta - y||_2 + \eta_X ||\beta - \gamma||_2.
$$

(5)

See proof in Appendix A.1.
In practice, Problem (5) will be solved by considering an equivalent form amenable to a simpler resolution in $\beta$ for any $\gamma$, that is:

$$
\min_{\beta \in \mathbb{R}^p} \max_{\gamma \in \mathcal{D}_\gamma} ||X\beta - y||_2^2 + \lambda ||\beta - \gamma||_2^2,
$$

(6)

where there is a one-to-one mapping between $\eta_X$ and $\lambda$. We now proceed to the definition of the uncertainty set $\mathcal{D}_\gamma$. Two options are proposed, each one entailing an equivalence with a well-known sparse regression method.

### 3. Assumptions on the Spurious Regression Coefficients

Though we envision several other applications of our framework, we present here two simple examples following the same pattern: assuming a given regularity on the regression coefficients $\beta^\star$, we consider the adversarial dual assumption on the spurious coefficients $\gamma$. When the initial regularity conditions on $\beta^\star$ are expressed by $\ell_1$ or $\ell_\infty$ norms, this process results in uncertainty sets $\mathcal{D}_\gamma$ which are convex polytopes that are easy to manage when solving Problem (6), since they can be defined as the convex hulls of a finite number possible perturbations.

The two sparsity-inducing penalizers presented below have a grouping effect. The elastic net implements this grouping without predefining the group structure: strongly correlated predictors tend to be in or out of the model together ([Zou and Hastie, 2005]). The $\ell_{\infty,1}$ group-Lasso that is presented subsequently is based on a prescribed group structure and favors regression coefficients with identical magnitude within activated groups.

#### 3.1 Elastic Net

As an introductory example, let us consider the regularity assumption stating that the $\ell_1$-norm of $\beta^\star$ should be small:

$$
\mathcal{H}^\text{Lasso}_{\beta^\star} = \{ \beta \in \mathbb{R}^p : ||\beta||_1 \leq \eta_\beta \}.
$$

The dual assumption is that the $\ell_\infty$-norm of $\gamma$ should be controlled, say:

$$
\mathcal{D}^\text{Lasso}_\gamma = \left\{ \gamma \in \mathbb{R}^p : \sup_{\beta \in \mathcal{H}^\text{Lasso}_{\beta^\star}} \gamma^T \beta \leq 1 \right\} = \{ \gamma \in \mathbb{R}^p : ||\gamma||_\infty \leq \eta_\gamma \} = \text{conv}\{\{-\eta_\gamma, \eta_\gamma\}^p\},
$$

where $\eta_\gamma = 1/\eta_\beta$ and $\text{conv}$ denotes convex hull, so that Problem (6) reads:

$$
\min_{\beta \in \mathbb{R}^p} \max_{\gamma \in \{-\eta_\gamma, \eta_\gamma\}^p} \left\{ ||X\beta - y||_2^2 + \lambda ||\beta - \gamma||_2^2 \right\}
$$

$$
\iff \min_{\beta \in \mathbb{R}^p} ||X\beta - y||_2^2 + 2\lambda \eta_\gamma ||\beta||_1 + \lambda ||\beta||_2^2,
$$

(7)

which is recognized as an elastic-net problem. When $\eta_\gamma$ is null, we recover ridge regression, and when the magnitude of $\eta_\gamma$ grows, the problem approaches a Lasso problem. A 2D
3.2 Group-Lasso

We consider here the $\ell_{\infty,1}$ variant of the group-Lasso, which was first proposed by Turlach et al. (2005) to perform variable selection in the multiple response setup, which is first detailed before introducing the general situation. Following the previous example, we now consider the regularity assumption stating that the $\ell_{\infty}$-norm of $\beta^*$ should be small:

$$H_{\beta^*}^{\text{Max}} = \{ \beta \in \mathbb{R}^p : ||\beta||_{\infty} \leq \eta_{\beta} \} .$$

The dual assumption is that the $\ell_1$-norm of $\gamma$ should be controlled:

$$D_{\gamma}^{\text{Max}} = \left\{ \gamma \in \mathbb{R}^p : \sup_{\beta \in H_{\beta^*}^{\text{Max}}} \gamma^T \beta \leq 1 \right\}$$

$$= \{ \gamma \in \mathbb{R}^p : ||\gamma||_1 \leq \eta_{\gamma} \}$$

$$= \text{conv} \{ \eta_{\gamma} e_1^p, \ldots, \eta_{\gamma} e_p^p, -\eta_{\gamma} e_1^p, \ldots, -\eta_{\gamma} e_p^p \} ,$$

where $\eta_{\gamma} = 1/\eta_{\beta}$ and $e_j^p$ is the $j$th element of the canonical basis of $\mathbb{R}^p$, that is $e_{jj'} = 1$ if $j = j'$ and $e_{jj'} = 0$ otherwise. Then, Problem (6) becomes:

$$\min_{\beta \in \mathbb{R}^p} \max_{\gamma \in D_{\gamma}^{\text{Max}}} \left\{ ||X\beta - y||_2^2 + \lambda ||\beta - \gamma||_2^2 \right\}$$

$$\Leftrightarrow \min_{\beta \in \mathbb{R}^p} ||X\beta - y||_2^2 + 2\lambda \eta_{\gamma} ||\beta||_{\infty} + \lambda ||\beta||_2^2 ,$$

Figure 1: Admissible sets (represented by colored patches) for the elastic-net. Here, these sets are defined by the intersection of the Euclidean balls whose centers are represented by crosses and boundaries are displayed in black.
Now, consider the more general situation where a group structure is defined on the set of variables by setting a partition of the index set $\mathcal{I} = \{1, \ldots, p\}$, that is,

$$
\mathcal{I} = \bigcup_{k=1}^{K} \mathcal{G}_k, \quad \text{with} \quad \mathcal{G}_k \cap \mathcal{G}_\ell = \emptyset \quad \text{for} \quad k \neq \ell.
$$

Let $p_k$ denote the cardinality of group $k$, and $\beta_{\mathcal{G}_k} \in \mathbb{R}^{p_k}$ be the vector $(\beta_j)_{j \in \mathcal{G}_k}$. We now consider the regularity assumption stating that the $\ell_\infty,1$ mixed-norm of $\beta^*$ (that is, its groupwise $\ell_\infty$-norm) should be small:

$$
\mathcal{H}_{\beta^*}^{\ell_\infty,1} = \left\{ \beta \in \mathbb{R}^p : \sum_{k=1}^{K} ||\beta_{\mathcal{G}_k}||_\infty \leq \eta_\beta \right\}.
$$

The dual assumption is that the groupwise $\ell_1$-norm of $\gamma$ should be controlled:

$$
\mathcal{D}_\gamma^{\ell_\infty,1} = \left\{ \gamma \in \mathbb{R}^p : \sup_{\beta \in \mathcal{H}_{\beta^*}^{\ell_\infty,1}} \gamma^T \beta \leq 1 \right\}
$$

$$
= \left\{ \gamma \in \mathbb{R}^p : \sum_{k=1}^{K} ||\gamma_{\mathcal{G}_k}||_1 \leq \eta_\gamma \right\}
$$

$$
= \text{conv}\left\{ \{\eta_\gamma e_{p_1}, \ldots, -\eta_\gamma e_{p_1}\}, \ldots, \{\eta_\gamma e_{p_K}, -\eta_\gamma e_{p_K}\} \right\},
$$

so that Problem (6) becomes:

$$
\min_{\beta \in \mathbb{R}^p} \max_{\gamma \in \mathcal{D}_\gamma^{\ell_\infty,1}} \left\{ ||X\beta - y||_2^2 + \lambda ||\beta - \gamma||_2^2 \right\}
$$

$$
\iff \min_{\beta \in \mathbb{R}^p} ||X\beta - y||_2^2 + 2\lambda \eta_\gamma \sum_{k=1}^{K} ||\beta_{\mathcal{G}_k}||_\infty + \lambda ||\beta||_2^2,
$$

Notice that the limiting cases of this penalty are two classical problems: ridge regression and the $\ell_\infty,1$ group-Lasso.

4. Algorithm

The unified derivation for the problems presented in Section 3 suggests a unified processing based on the iterative resolution of quadratic problems. Our algorithm is summarized in this section. We then describe an alternative to Fenchel duality (used for example by Bach et al., 2012) to assess convergence, by computing an upper-bound for the gap between the current solution and the optimal one.

4.1 Active Set Approach

The efficient approaches developed for sparse regression take advantage of the sparsity of the solution by solving a series of small linear systems, whose sizes are incrementally
increased/decreased. Here, as for the Lasso (Osborne et al., 2000; Efron et al., 2004), this process boils down to an iterative optimization scheme involving the resolution of quadratic problems.

The algorithm starts from a sparse initial guess, say $\beta = 0$, and iterates the three following steps:

1. the first step solves Problem (6) with respect to $\beta_A$, the subset of “active” variables, currently identified as being non-zero. This penalized least squares problem is defined from $X_A$, which is the submatrix of $X$ comprising all rows and the columns indexed by $A$ and $\gamma_A$, which is set to its current most adversarial value.

2. the second step updates $\beta_A$ if necessary (and possibly $\gamma_A$), so that $\gamma_A$ is indeed (one of) the most adversarial value of the current $\beta_A$. This is easily checked with the problems given in Section 3, where $D_\gamma$ is a convex polytope whose vertices (that is, extreme $\gamma$-values) are associated with a cone of coherent $\beta$-value.

3. the last step updates the active set $A$. It relies on the "worst-case gradient" with respect to $\beta$, where $\gamma$ is chosen so as to minimize infinitesimal improvements of the current solution. Again picking the right $\gamma$ is easy for the problems given in Section 3. Once this is done, we first check whether some variables should quit the active set, and if this is not the case, we assess the completeness of $A$, by checking the optimality conditions with respect to inactive variables. We add the variable, or the group of variables that most violates the worst-case optimality conditions. When no such violation exists, the current solution is optimal, since, at this stage, the problem is solved exactly within the active set $A$.

Algorithm 1 provides a more comprehensive technical description. Note that the structure is essentially identical to the one proposed by Osborne et al. (2000) or Efron et al. (2004) for the Lasso. The viewpoint is however radically different, as the global non-smooth problem

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2. When several $\gamma_A$ are equally unfavorable to $\beta_A$, we use gradient information to pick the worst one among those when $\beta_A$ moves along the steepest descent direction.
Algorithm 1: Worst-Case Quadratic Penalty Active Set Algorithm

Init. $\beta \leftarrow \beta^0$
- Determine the active set: $\mathcal{A} \leftarrow \{j : \beta > 0\}$
- Pick a worst admissible $\gamma$, that is, $\gamma = \arg \max_{g \in \mathcal{D}_\gamma} ||\beta - g||^2_2$

Step 1 Update active variables $\beta_A$ assuming that $A$ and $\gamma_A$ are optimal

$\beta_A^{old} \leftarrow \beta_A$

$\beta_A \leftarrow (X_A^T X_A + \lambda I_{|A|})^{-1} (X_A^T y + \lambda \gamma_A)$

Step 2 Verify coherence of $\gamma_A$ with the updated $\beta_A$

if $||\beta_A - \gamma_A||^2 < \max_{g \in \mathcal{D}_\gamma} ||\beta_A - g||^2$ then // if $\gamma_A$ is not worst-case

/* Backtrack towards the last $\gamma_A$-coherent solution: */

$\beta_A \leftarrow \beta_A^{old} + \rho (\beta_A - \beta_A^{old})$

$\gamma_A$ is worst-case for $\beta_A$, and there is another worst-case value $\tilde{\gamma}_A$

/* Check whether progress can be made with $\tilde{\gamma}_A$ */

$\tilde{\beta}_A \leftarrow (X_A^T X_A + \lambda I_{|A|})^{-1} (X_A^T y + \lambda \tilde{\gamma}_A)$

if $||\tilde{\beta}_A - \tilde{\gamma}_A||^2_2 = \max_{g \in \mathcal{D}_\gamma} ||\beta_A - g||^2_2$ then // if $\tilde{\gamma}_A$ is worst-case...

$(\beta_A, \gamma_A) \leftarrow (\tilde{\beta}_A, \tilde{\gamma}_A)$ // $(\beta_A, \gamma_A)$ is better than $(\beta_A, \gamma_A)$

/* The current $\gamma_A$ is coherent with $\beta_A$ */

Step 3 Update active set $A$

$g_j \leftarrow \min_{\gamma \in \mathcal{D}_\gamma} |X_A^T (X_A \beta_A - y) + \lambda (\beta_j - \gamma_j)| \quad j = 1, \ldots, p$ // worst-case gradient

if $\exists j \in A : \beta_j = 0$ and $g_j = 0$ then

$A \leftarrow A \backslash \{j\}$; // Downgrade $j$

/* Go to Step 1 */

else

if $\max_{j \in A^c} g_j \neq 0$ then

/* Identify the greatest violation of optimality conditions: */

$j^* \leftarrow \arg \max_{j \in A^c} g_j, \quad A \leftarrow A \cup \{j^*\}$; // Upgrade $j^*$

/* Go to Step 1 */

else

/* Stop and return $\beta$, which is optimal */

is dealt with subdifferentials by Osborne et al. (2000), whereas we rely on the maximum of smooth functions, suggesting the assessment of convergence detailed below.

4.2 Monitoring Convergence

At each iteration of the algorithm, the current $\beta$ is computed assuming that the current active set $A$ and the current $\gamma_A$-value are optimal. When the current active set is not optimal, the current $\beta$ (where $\beta_A$ is completed by zeros on the complement $A^c$) is never-
theless optimal for a \( \gamma \)-value defined in \( \mathbb{R}^p \) (where \( \gamma_A \) is completed by ad hoc values on the complement \( A^c \)). However this \( \gamma \) fails to belong to \( D_\gamma \) (otherwise, the problem would be solved: \( A, \gamma \) and \( \beta \) would indeed be optimal). The following proposition relates the current objective function, associated with an infeasible \( \gamma \)-value (\( \gamma \notin D_\gamma \)), to the global optimum of the optimization problem.

**Proposition 2** For any \( \eta_\gamma > 0 \), and for all vectorial norm \( \|\cdot\|_* \), when \( D_\gamma \) is defined as

\[
D_\gamma = \{ \gamma \in \mathbb{R}^p : \|\gamma\|_* \leq \eta_\gamma \},
\]

then, \( \forall \gamma \in \mathbb{R}^p : \|\gamma\|_* \geq \eta_\gamma \), we have:

\[
\min_{\beta \in \mathbb{R}^p} \max_{\gamma' \in D_\gamma} J_\lambda(\beta, \gamma') \geq \frac{\eta_\gamma}{\|\gamma\|_*} J_\lambda(\beta^*(\gamma), \gamma) - \frac{\lambda \eta_\gamma (\|\gamma\|_* - \eta_\gamma)}{\|\gamma\|_*^2} \|\gamma\|_*^2,
\]

where

\[
J_\lambda(\beta, \gamma) = \|X\beta - y\|_2^2 + \lambda \|\beta - \gamma\|_2^2 \quad \text{and} \quad \beta^*(\gamma) = \arg \min_{\beta \in \mathbb{R}^p} J_\lambda(\beta, \gamma).
\]

See proof in Appendix A.2.

This proposition can be used to compute an optimality gap at Step 3 of Algorithm 1 by picking a \( \gamma \)-value such that the current worst-case gradient \( g \) is null (the current \( \beta \)-value then being the optimal \( \beta^*(\gamma) \)). Other options could be considered, but they would result in significant extra computation. The optimality gap computed from Proposition 2 differs from the Fenchel duality gap (see Bach et al., 2012). For the elastic net expressed in (7), Fenchel inequality (see details in Mairal, 2010) yields the following optimality gap:

\[
\min_{\beta \in \mathbb{R}^p} \max_{\gamma' \in D_\gamma} J_\lambda(\beta, \gamma') \geq \frac{\eta_\gamma}{\|\gamma\|_*} \left( \|X\beta^*(\gamma) - y\|_2^2 + \lambda \|\beta^*(\gamma)\|_2^2 \right) - 2 \frac{\eta_\gamma}{\|\gamma\|_*} (X\beta^*(\gamma) - y)^T y.
\]

The two optimality gaps are empirically compared in Figure 3 for the elastic net, along a short regularization path with five values of the \( \ell_1 \)-penalization parameter. Fenchel’s duality gap is more accurate here, especially for the rougher solutions. However, the practical use of these upper bounds is rather limited as they are both fairly coarse unless a very accurate solution is reached. These optimality gaps may thus be used to assess convergence, but they are ineffective as stopping rules when fast and rough solutions are sought.

### 5. Numerical Experiments

This section compares the performances of our algorithm to its state-of-the-art competitors from an optimization viewpoint. Efficiency may then be assessed by accuracy an speed: accuracy is the difference between the optimum of the objective function and its value at the solution returned by the algorithm; speed is the computing time required for returning this solution. Obviously, the timing of two algorithms/packages has to be compared at similar precision requirements, which are rather crude in machine learning, far from machine precision (Bottou and Bousquet, 2008).
We compare the performance of the proposed quadratic solver with representatives of the most successful competing algorithms. First, we use our own implementations of all competitors, so as to provide comparisons without implementation biases (language, library, etc.). We use R with most of the matrix calculus done in C++ using the RcppArmadillo package (Eddelbuettel and François [2011], Sanderson [2010]) that relies on BLAS/LAPACK libraries for linear algebra operations. Second, we compare our code to the leading standalone packages that are available today, so as to provide comparisons avoiding a possible competence bias.

We use simulated data to obtain representative average results. Their generation covers the typical attributes of the real data encountered in post genomic and signal processing. In these domains, the main optimization difficulties result from ill-conditioning, which is either due to the high correlation between predictors, or to underdetermination when the number of variables exceeds the sample size (also known as the high-dimensional or the “large p small n” setup). For the optimization algorithms based on active set strategies, bad conditioning is somehow alleviated when the objective function has a regular behavior when restricted to the subspace containing the solution. All other things being equal, this local conditioning is thus governed by the sparsity of the unknown true parameter (which affects the sparsity of the solution), which also heavily impacts the running times of most optimization algorithms available today.
5.1 Data Generation

The above-mentioned characteristics are explored without difficulty in the framework of linear regression. We generate samples of size $n$ from the model

$$y = X\beta^* + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I),$$

with $\sigma$ chosen so as to reach a rather strong coefficient of determination ($R^2 \approx 0.8$). The design matrix $X$ is drawn from a multivariate normal distribution in $\mathbb{R}^p$, and the conditioning of $X^\top X$ is ruled by the correlation between variables. We use the same correlation coefficient $\rho$ for all pairs of variables. The sparsity of the true regression coefficients is controlled by a parameter $s$, with

$$\beta^* = \left(\frac{2}{s/2}, \ldots, -\frac{2}{s/2}, \ldots, -\frac{2}{s/2}, 0, \ldots, 0\right).$$

Finally, the ratio $p/n$ quantifies the well/ill-posedness of the problem.

5.2 Comparing Optimization Strategies

We compare here the performance of three state-of-the-art optimization strategies implemented in our own computational framework: accelerated proximal method (see, e.g., Beck and Teboulle, 2009), coordinate descent (popularized by Friedman et al., 2007), and our algorithm, that will respectively be named hereafter proximal, coordinate and quadratic. Our implementations estimate the solution to elastic-net problem

$$J_{\lambda_1, \lambda_2}^{\text{enet}}(\beta) = \frac{1}{2} ||X\beta - y||^2_2 + \lambda_1 ||\beta||_1 + \frac{\lambda_2}{2} ||\beta||^2_2,$$

which is strictly convex when $\lambda_2 > 0$ and thus admits a unique solution even if $n < p$.

The three implementations are embedded in the same active set routine, which approximately solves the optimization problem with respect to a limited number of variables as in Algorithm 1. They only differ regarding the inner optimization problem with respect to the current active variables, which is performed by an accelerated proximal gradient method for proximal, by coordinate descent for coordinate, and by the resolution of the worst-case quadratic problem for quadratic. We followed the practical recommendations of Bach et al. (2012) for accelerating the proximal and coordinate descent implementations, and we used the same halting condition for the three implementations, based on the approximate satisfaction of the first-order optimality conditions:

$$\max_{j \in \{1, \ldots, p\}} \left| x_j^\top \left( y - X\hat{\beta} \right) + \lambda_2 \hat{\beta} \right| < \lambda_1 + \tau,$$

where the threshold $\tau$ was fixed to $\tau = 10^{-2}$ in our simulations. Finally, the active set algorithm is itself wrapped in a warm-start routine, where the approximate solution to $J_{\lambda_1, \lambda_2}^{\text{enet}}$ is used as the starting point for the resolution of $J_{\lambda_1', \lambda_2}^{\text{enet}}$ for $\lambda_1' < \lambda_1$.

Our benchmark considers small-scale problems, with size $p = 100$, and the nine situations stemming from the choice of three following parameters:

3. The rather loose threshold is favorable to coordinate and proximal, which reach the threshold, while quadratic ends up with a much smaller value, due to the exact resolution, up to machine precision, of the inner quadratic problem.
• low, medium and high levels of correlation between predictors ($\rho \in \{0.1, 0.4, 0.8\}$),
• low, medium and high-dimensional setting ($p/n \in \{2, 1, 0.5\}$),
• low, medium and high levels of sparsity ($s/p \in \{10\%, 30\%, 60\%\}$).

Each solver computes the elastic net for the tuning parameters $\lambda_1$ and $\lambda_2$ on a 2D-grid of $50 \times 50$ values, and their running times have been averaged over 100 runs.

All results are qualitatively similar regarding the dimension and sparsity settings. Figure 4 displays the high-dimensional case ($p = 2n$) with a medium level of sparsity ($s = 30$) for the three levels of correlation. Each map represents the log-ratio between the timing of either coordinate or proximal versus quadratic, according to $(\lambda_1, \lambda_2)$ for a given correlation level. Dark regions with a value of 1 indicate identical running times while lighter regions with a value of 10 indicate that quadratic is 10 times faster. Figure 4 illustrates that quadratic outperforms both coordinate and proximal, by running much faster in most cases, even reaching 300-fold speed increases. The largest gains are observed for small $(\lambda_1, \lambda_2)$ penalty parameters for which the problem is ill-conditioned, including many active variables, resulting in a huge slowdown of the first-order methods coordinate and proximal. As the penalty parameters increase, smaller gains are observed, especially when $\lambda_2$, attached to the quadratic penalty, reaches high values for which all problems are well-conditioned, and where the elastic-net is leaning towards univariate soft thresholding, in which case all algorithms behave similarly.

5.3 Comparing Stand-Alone Implementations

We now proceed to the evaluation of our code with three other stand-alone programs publicly available as R packages. We chose three leading state-of-the-art packages, namely glmnet (Generalized Linear Models regularized by Lasso and elastic-NET, Friedman et al., 2010), lars (Least Angle Regression, lasso and forward Stagewise, Efron et al., 2004) and SPAMS (SPArse Modeling Software, Bach et al., 2012), with two options SPAMS-FISTA, which implements an accelerated proximal method, and SPAMS-LARS which is a lars substitute. Note that glmnet does most of its internal computations in Fortran, lars in R, and SPAMS in C++. Our own implementation, by resolution of worst-case quadratic problem, is shipped within an R package quadrupen publicly available at the second author’s web page.4

We benchmark these packages by computing regularization paths for the Lasso, that is, the elastic-net Problem (8) with $\lambda_2 = 0$. The inaccuracy of the solutions produced is measured by the gap in the objective function compared to a reference solution, considered as being the true optimum. We use the lars solution as a reference, since it solves the Lasso problem up to the machine precision, relying on the LAPACK/BLAS routines. Furthermore, lars provides the solution path for the Lasso, that is, the set of solutions computed for each penalty parameter value for which variable activation or deletion occurs, from the empty model to the least-mean squares model. This set of reference penalty parameters is used here to define a sensible reproducible choice.

4. or directly at http://stat.genopole.cnrs.fr/logiciels/quadrupen. This will be made available on the CRAN (Comprehensive R Archive Network)
5. We benchmark the packages on a Lasso problem since the parametrization of the elastic-net problem differs among packages, hindering fair comparisons.
Figure 4: Log-ratio of computation times for coordinate (left), and proximal (right), versus quadratic, for \((p, n) = (100, 50), s = 30\) and correlation \(\rho \in \{0.1, 0.4, 0.8\}\) (top, middle and bottom respectively).
In high dimensional setups, the computational cost of returning the solutions for the largest models may be overwhelming compared to the one necessary for exploring the interesting part of the regularization path \cite{Simon11,Friedman10}. This is mostly due to numerical instability problems that may be encountered in these extreme settings, where the Lasso solution is overfitting as it approaches the set of solutions to the underdetermined least squares problem. We avoid a comparison mostly relying on these spurious cases by restricting the set of reference penalty parameters to the first $\min(n,p)$ steps of \texttt{lars} \cite{Friedman10}.

Henceforth, the distance $D$ of a given \texttt{method} to the optimum is evaluated on the whole set of penalties $\Lambda$ used along the path, by

$$D(\text{method}) = \left( \frac{1}{|\Lambda|} \sum_{\lambda \in \Lambda} \left( J_{\lambda}^{\text{lasso}} \left( \hat{\beta}_\lambda^{\text{lars}} \right) - J_{\lambda}^{\text{lasso}} \left( \hat{\beta}_\lambda^{\text{method}} \right) \right)^2 \right)^{1/2},$$

where $J_{\lambda}^{\text{lasso}}(\beta) = J_{\lambda,0}^{\text{enet}}(\beta)$ is the objective function of the Lasso evaluated at $\beta$, and $\hat{\beta}_\lambda^{\text{method}}$ is the estimated optimal solution provided by the \texttt{method} package currently tested.

The data sets are generated according to the linear model described above, in three different high-dimensional settings and small to medium number of variables: $(p,n) = (100,40), (p,n) = (1000,200)$ and $(p,n) = (10000,400)$. The sparsity of the true underlying $\beta^*$ is governed by $s = 0.25 \min(n,p)$, and the correlation between predictors is set by $\rho \in \{0.1,0.4,0.8\}$. For each value of $\rho$, we averaged the timings over 50 simulations, ensuring that each package computes the solutions at identical $\lambda$ values, as defined above.

We pool together the runtimes obtained for the three levels of correlation for \texttt{quadrupen}, \texttt{SPAMS-LARS} and \texttt{lars}, which are not sensible to the correlation between features. In each plot of Figure 5 each of these methods is thus represented by a single point marking the average precision and the average distance to the optimum over the 150 runs (50 runs for each $\rho \in \{0.1,0.4,0.8\}$). Note that for \texttt{lars} only the abscissa is meaningful since $D(\text{lars})$ is zero by definition. Besides, \texttt{quadrupen}, which solves each quadratic problem up to the machine precision, tends to be within this precision of the \texttt{lars} solution. The \texttt{SPAMS-LARS} is also very precise, up to $10^{-6}$, which is the typical precision of the approximate resolution of linear systems. It is the fastest alternative for solving the Lasso when the problem is high-dimensional with a large number of variables (Figure 5, bottom-left).

In contrast, the (precision,timing)-values of \texttt{glmnet} and \texttt{SPAMS-FISTA} are highly affected by the threshold parameters that control their stopping conditions. The computational burden to reach a given precision is also affected by the level of correlation, as illustrated in Figure 5. Obviously, a precise solution is difficult to reach with first-order descent algorithms in a high correlation setup, which corresponds to an ill-conditioned linear system. It may be surprising to observe that \texttt{SPAMS-FISTA} is about ten time slower than \texttt{glmnet}, as proximal and coordinate descent methods were experimentally shown to be roughly equivalent in our preceding analysis and by \cite{Bach12}. However, these two comparisons were carried out with the same active set strategy (that is, with active set for ours and without active

\footnote{In \texttt{glmnet}, convergence is monitored by the stability of the objective function, measured between two optimization steps, and optimization is halted when changes fall below the specified threshold (scaled by the null deviance). In \texttt{SPAMS-FISTA}, the stopping condition of the algorithm is based on the relative change of parameters between two iterations.}
Figure 5: Distance to optimum versus CPU time for three different high-dimensional settings: \((p, n) = (100, 40)\) (top left), \((p, n) = (1000, 200)\) (top right) and \(p = (10000, 400)\) (bottom left).
We believe that this difference in the handling of active variables explains the relative bad performance of \texttt{SPAMS-FISTA}, which optimizes all variables along the regularization path, while \texttt{glmnet} uses a greedy active set strategy.

Overall, our implementation is highly competitive, that is, very accurate, at the \texttt{lars} level, and much faster. The speed improvements of \texttt{glmnet} are only observed for very rough approximate solutions and \texttt{SPAMS-FISTA} is dominated by \texttt{glmnet}. Our experiments, in the framework of active set methods, agree with the results of Bach et al. (2012): indeed, they observed that first-order methods are competitive with second-order ones only for low correlation levels and small penalties (which entails a large number of active variables). Conversely, our results may appear to contradict some of the experimental findings of Friedman et al. (2010): first, we observe that \texttt{glmnet} is quite sensitive to correlations, and second, the optimized second-order methods are competitive with \texttt{glmnet}. These differences in conclusions arise from the differences in experimental protocols: while we compare running times at a given accuracy, they are compared at a given threshold on the stopping criterion by Friedman et al. (2010). Regarding the influence of correlations, the stability-based criterion can be fooled due to the tiny step size that typically occurs for ill-conditioned problems, leading to a sizable early stopping. Regarding the second point, even though the \texttt{R} implementation of \texttt{lars} may indeed be slow compared to \texttt{glmnet}, considerable improvements can be obtained using optimized second-order methods such as \texttt{quadrupen} as soon as a sensible accuracy is required, especially when correlation increases.

Finally, among the accurate solvers, \texttt{SPAMS-LARS} is insignificantly less accurate than \texttt{quadrupen} or \texttt{lars} in a statistical context. It is always faster than \texttt{lars} and slightly faster than \texttt{quadrupen} for the largest problem sizes (Figure 5, bottom-left) and much slower for the smallest problem (Figure 5, top-left).

### 5.4 Link between accuracy of solutions and prediction performances

When the “irrepresentable condition” (Zhao and Yu, 2006) holds, the Lasso should select the true model consistently. However, even when this rather restrictive condition is fulfilled, perfect support recovery obviously requires numerical accuracy: rough estimates may speed up the procedure, but whatever optimization strategy is used, stopping an algorithm is likely to prevent either the removal of all irrelevant coefficients or the insertion of all relevant ones. The support of the solution may then be far from the optimal one.

We advocate here that our quadratic solver is very competitive in computation time when support recovery matters, that is, when high level of accuracy is needed, in small (few hundreds of variables) and medium sized problems (few thousands). As an illustration, we generate 100 data sets under the same linear model as above, with a rather strong coefficient of determination ($R^2 \approx 0.8$ on average), a rather high level of correlation between predictors ($\rho = 0.8$) and a medium level of sparsity ($s/p = 30\%$). The number of variable is kept low ($p = 100$) and the difficulty of the problem is tuned by the $n/p$ ratio. For each data set, we also generate a test set sufficiently large (say, $10n$) to evaluate the quality of the prediction without depending on any sampling fluctuation. We compare the Lasso solutions computed
by quadrupen to the ones returned by glmnet with various level of accuracy\footnote{This is done via the \texttt{thresh} argument of the \texttt{glmnet} procedure, whose default value is $1e^{-7}$. In our experiments, \texttt{low}, \texttt{med} and \texttt{high} level of accuracy for \texttt{glmnet} respectively correspond to \texttt{thresh} set to $1e^{-1}$, $1e^{-4}$, and $1e^{-9}$.} Figure 6 reports performances, as measured by the mean squared test error and the support error rate.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6}
\caption{Test performances according to the penalty parameter for the Lasso estimates returned by quadrupen and glmnet at various level of accuracy. Three high-dimensional setups are illustrated: from left to right $n/p = 1/2$, $n/p = 1$ and $n/p = 2$; top: mean squared test error; bottom: support error rate.}
\end{figure}
As expected, the curves show that selecting variables and searching for the best prediction are two different problems. The selection problem (bottom of Figure 6) always requires a sparser model than the prediction problem. But despite this obvious difference, the more accurate the solution returned by the algorithm, the better the performances for any levels of penalty and for both performance measures.

| methods       | quadupen | glmnet (low) | glmnet (med) | glmnet (high) |
|---------------|----------|--------------|--------------|--------------|
| timing (ms)   | 8        | 7            | 8            | 64           |
| accuracy (dist. to opt.) | $5.9 \times 10^{-14}$ | $7.2 \times 10^0$ | $6.04 \times 10^0$ | $1.47 \times 10^{-2}$ |

Table 1: Median timings and solution accuracies

Now focusing on glmnet performances, the better the accuracy, the smaller the MSE and the support error rate. But the better the accuracy, the slower the algorithm becomes. Using the default settings allows to have a result very close to our quadratic solver, and the performance differences become negligible between our approach and glmnet running with high precision. However, Table 1 illustrates that high accuracy is achieved at a high computational cost: to be at par with quadupen with regards to test performances, glmnet is about ten times slower than our solver.

6. Discussion

This paper presents a new viewpoint on sparsity-inducing penalties stemming from robust optimization. This viewpoint enables to cast in the same framework several well-known penalties, to derive a general-purpose algorithm that computes the solution to their companion penalized regression problem, and to obtain a lower bound on the minimum of the objective function that provides an assessment of convergence. The proposed algorithm solves a series of small-size quadratic problems defined from the currently estimated worst-case perturbation. It has been thoroughly tested and compared with state-of-the-art implementations for the elastic net and the Lasso, comparing favorably in most cases to all its competitors.

We detailed here how the Lasso and the group-Lasso (with the $\ell_{\infty,1}$ mixed norm) penalties, possibly applied together with an $\ell_2$ ridge penalty (leading to what is known as the elastic net for the Lasso) can be derived from this new robust optimization viewpoint. The algorithm can be adapted to non-quadratic loss functions for addressing other learning problems such as classification, but this generalization, which requires solving non-quadratic problems, may not be as efficient compared to the existing alternatives. We are now examining how to address a wider range of penalties by extending the framework in two directions: first, to accommodate additional general $\ell_2$ penalties in the form of arbitrary symmetric positive semidefinite matrix instead of the simple ridge, in particular to provide an efficient implementation of the structured elastic-net [Slawski et al.] [2010]; second, we plan to derive similar views on a wider range of sparsity-inducing penalties, such as the fused-Lasso or the OSCAR [Bondell and Reich 2008].

Acknowledgments
Appendix A. Proofs

A.1 Proof of Proposition 1

First show that the objective function of Problem (4) is, up to an irrelevant constant, upper bounded by the objective function of Problem (5):

\[ \| (X - \Delta X)\beta + X\gamma + \epsilon - y \|_2 \leq \| X(\beta + \gamma) - y \|_2 + \| \Delta X \beta \|_2 + \| \epsilon \|_2 \]

(10)

\[ \leq \| X(\beta + \gamma) - y \|_2 + \eta_X \| \beta \|_2 + \eta_\epsilon \]

(11)

where (10) stems from the triangular inequality and (11) follows from the definition of the uncertainty sets. The right-hand side of (11) is, up to an irrelevant constant, identical to the objective function of Problem (5) after the change of variable \( \beta \leftarrow \beta + \gamma \).

We conclude, by showing that, for all \((\beta, \gamma)\), there is \((\Delta X^*, \epsilon^*) \in \mathcal{D}_X \times \mathcal{D}_\epsilon\) such that the upper bound on the right-hand side of (11) is reached:

\[ \Delta X^* = \eta_X \frac{X(\beta + \gamma) - y}{\| X(\beta + \gamma) - y \|_2} \quad \epsilon^* = \eta_\epsilon \frac{X(\beta + \gamma) - y}{\| X(\beta + \gamma) - y \|_2} \]

With these choices, the vectors \(X(\beta + \gamma) - y, \Delta X^*\beta\) and \(\epsilon^*\) are colinear, so that minimizing the left-hand-side of (10) is equivalent to minimize the right-hand-side of (11).

A.2 Proof of Proposition 2

We detail here a proof yielding a slightly tighter bound. Proposition 2 is simply a corollary of Proposition 4 stated and proved below.

When \(\mathcal{D}_\gamma\) is defined by a norm as in Proposition 2, the following Lemma relates the penalty associated with a infeasible \(\gamma\)-value \(\| \gamma \|_\alpha > \eta_\gamma\) to the one obtained by shrinking this \(\gamma\)-value to reach the boundary of \(\mathcal{D}_\gamma\).

Lemma 3 Let \(S \subseteq \{1, \ldots, p\} \), \(\alpha \in (0, 1), \| \cdot \|_\alpha\) be a vectorial norm and \(\varphi^*(\cdot, S, \alpha) : \mathbb{R}^p \rightarrow \mathbb{R}^p\) be defined as follows:

\[ \begin{cases} 
\varphi^*_S(\gamma, S, \alpha) = \gamma_S \\
\varphi^*_S(\gamma, S, \alpha) = \alpha \gamma_{S^c} 
\end{cases} \]

Then,

\[ \| \beta - \varphi^*(\gamma, S, \alpha) \|_2^2 \geq \alpha \| \beta - \gamma \|_2^2 - \alpha(1 - \alpha) \| \gamma_{S^c} \|_2^2 \]

(12)

Proof

\[ \| \beta - \varphi^*(\gamma, S, \alpha) \|_2^2 = \| \beta_S - \gamma_S \|_2^2 + \alpha \| \beta_{S^c} - \gamma_{S^c} \|_2^2 + (1 - \alpha) \| \beta_{S^c} - \gamma_{S^c} \|_2^2 - \alpha(1 - \alpha) \| \gamma_{S^c} \|_2^2 \]

\[ \geq \| \beta_S - \gamma_S \|_2^2 + \alpha \| \beta_{S^c} - \gamma_{S^c} \|_2^2 - \alpha(1 - \alpha) \| \gamma_{S^c} \|_2^2 \]

\[ \geq \alpha \| \beta - \gamma \|_2^2 - \alpha(1 - \alpha) \| \gamma_{S^c} \|_2^2 \].
Proposition 4 For any $\eta_\gamma > 0$, and for all vectorial norm $||\cdot||_*$, when $D_\gamma$ is defined as $D_\gamma = \{\gamma \in \mathbb{R}^p : ||\gamma||_* \leq \eta_\gamma\}$, then, $\forall \gamma \in \mathbb{R}^p : ||\gamma||_* \geq \eta_\gamma$, and $\forall (S, \alpha) \in 2^{\{1, \ldots, p\}} \times (0, 1)$ such that $||(\gamma_S, \alpha \gamma_S^c)||_* \leq \eta_\gamma$, we have:

$$\min_{\beta \in \mathbb{R}^p} \max_{\gamma' \in D_\gamma} J_\lambda(\beta, \gamma') \geq \alpha J_\lambda(\beta^*(\gamma), \gamma) - \lambda \alpha(1 - \alpha) ||\gamma_S^c||^2_2,$$

where

$$J_\lambda(\beta, \gamma) = ||X\beta - y||^2_2 + \lambda ||\beta - \gamma||^2_2 \quad \text{and} \quad \beta^*(\gamma) = \arg \min_{\beta \in \mathbb{R}^p} J_\lambda(\beta, \gamma).$$

Proof For all $\beta \in \mathbb{R}^p$ and for any $(\gamma, S, \alpha) \in \mathbb{R}^p \times 2^{\{1, \ldots, p\}} \times (0, 1)$ such that $\varphi^*(\gamma, S, \alpha) \in D_\gamma$, with $\varphi^*$ defined as in Lemma 3 we have:

$$\max_{\gamma' \in D_\gamma} J_\lambda(\beta, \gamma') \geq J_\lambda(\beta, \varphi^*(\gamma, S, \alpha)),$$

(13)

since $\varphi^*(\gamma, S, \alpha)$ belongs to $D_\gamma$. We now compute a lower bound of the right-hand-side for $\gamma$ such that $||\gamma||_* \geq \eta_\gamma$:

$$J_\lambda(\beta, \varphi^*(\gamma, S, \alpha)) = \alpha \left( \frac{1}{\alpha} ||X\beta - y||^2_2 + \frac{\lambda}{\alpha} ||\beta - \varphi^*(\gamma, S, \alpha)||^2_2 \right) \geq \alpha \left( ||X\beta - y||^2_2 + \frac{\lambda}{\alpha} ||\beta - \varphi^*(\gamma, S, \alpha)||^2_2 \right) \geq \alpha \left( ||X\beta - y||^2_2 + \lambda ||\beta - \gamma||^2_2 \right) - \lambda \alpha(1 - \alpha) ||\gamma_S^c||^2_2,$$

where the last inequality stems from Lemma 3. This inequality holds for any given $\beta$-value, in particular for $\beta^*(\varphi^*(\gamma, S, \alpha)) = \arg \min_{\beta \in \mathbb{R}^p} J_\lambda(\beta, \varphi^*(\gamma, S, \alpha))$:

$$\min_{\beta \in \mathbb{R}^p} J_\lambda(\beta, \varphi^*(\gamma, S, \alpha)) \geq \alpha J_\lambda(\beta^*(\varphi^*(\gamma, S, \alpha))) - \lambda \alpha(1 - \alpha) ||\gamma_S^c||^2_2 \geq \alpha J_\lambda(\beta^*(\gamma), \gamma) - \lambda \alpha(1 - \alpha) ||\gamma_S^c||^2_2,$$

(14)

where the second inequality follows from the definition of $\beta^*(\gamma)$. Inequality (14) can be restated as:

$$\min_{\beta \in \mathbb{R}^p} J_\lambda(\beta, \varphi^*(\gamma, S, \alpha)) \geq \alpha \min_{\beta \in \mathbb{R}^p} J_\lambda(\beta, \gamma) - \lambda \alpha(1 - \alpha) ||\gamma_S^c||^2_2.$$

We finally remark that, since $\varphi^*(\gamma, S, \alpha) \in D_\gamma$, we trivially have:

$$\min_{\beta \in \mathbb{R}^p} \max_{\gamma' \in D_\gamma} J_\lambda(\beta, \gamma') \geq \min_{\beta \in \mathbb{R}^p} J_\lambda(\beta, \varphi^*(\gamma, S, \alpha)),$$

which concludes the proof. 

\[ \Box \]
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