

Simultaneous Regression Shrinkage, Variable Selection, and Supervised Clustering of Predictors with OSCAR

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SUMMARY. Variable selection can be challenging, particularly in situations with a large number of predictors with possibly high correlations, such as gene expression data. In this article, a new method called the OSCAR (octagonal shrinkage and clustering algorithm for regression) is proposed to simultaneously select variables while grouping them into predictive clusters. In addition to improving prediction accuracy and interpretation, these resulting groups can then be investigated further to discover what contributes to the group having a similar behavior. The technique is based on penalized least squares with a geometrically intuitive penalty function that shrinks some coefficients to exactly zero. Additionally, this penalty yields exact equality of some coefficients, encouraging correlated predictors that have a similar effect on the response to form predictive clusters represented by a single coefficient. The proposed procedure is shown to compare favorably to the existing shrinkage and variable selection techniques in terms of both prediction error and model complexity, while yielding the additional grouping information.

KEY WORDS: Correlation; Penalization; Predictive group; Regression; Shrinkage; Supervised clustering; Variable selection.

1. Introduction

Variable selection for regression models with many covariates is a challenging problem that permeates many disciplines. Selecting a subset of covariates for a model is particularly difficult if there are groups of highly correlated covariates. As a motivating example, consider a recent study of the association between soil composition and forest diversity in the Appalachian Mountains of North Carolina. For this study, there are 15 soil characteristics potentially to be used as predictors, of which there are 7 that are highly correlated. Based on a sample of 20 forest plots, the goal is to identify the important soil characteristics.

Penalized regression has emerged as a highly successful technique for variable selection. For example, the least absolute shrinkage and selection operator (LASSO; Tibshirani, 1996) imposes a bound on the L_1 norm of the coefficients. This results in both shrinkage and variable selection due to the nature of the constraint region, which often results in several coefficients becoming identically zero. However, a major stumbling block for the LASSO is that if there are groups of highly correlated variables, it tends to arbitrarily select only one from each group. These models are difficult to interpret because covariates that are strongly associated with the outcome are not included in the predictive model.

Supervised clustering, or determining meaningful groups of predictors that form predictive clusters, can be beneficial in both prediction and interpretation. In the soil data, several of the highly correlated predictors are related to the same underlying factor, the abundance of positively charged ions, and

hence can be combined into a group. However, just combining them beforehand can dilute the group's overall signal, as not all of them may be related to the response in the same manner. As another example, consider a gene expression study in which several genes sharing a common pathway may be combined to form a grouped predictor. For the classification problem in which the goal is to discriminate between categories, Jörnsten and Yu (2003) and Dettling and Bühlmann (2004) perform supervised gene clustering along with subject classification. These techniques are based on creating a new predictor, which is just the average of the grouped predictors, called a "super gene" for gene expression data by Park, Hastie, and Tibshirani (2007). This form of clustering aids in prediction as the process of averaging reduces the variance. It also suggests a possible structure among the predictor variables that can be further investigated.

For a continuous response, Hastie et al. (2001) and Park et al. (2007) first perform hierarchical clustering on the predictors, and, for each level of the hierarchy, take the cluster averages as the new set of potential predictors for the regression. After clustering, the response is then used to select a subset of these candidate grouped predictors via either stepwise selection or using the LASSO.

An alternative and equivalent view of creating new predictors from the group averages is to consider each predictor in a group as being assigned identical regression coefficients. This article takes this alternative point of view, which allows supervised clustering to be directly incorporated into the estimation procedure via a novel penalization method. The new

method called the OSCAR (octagonal shrinkage and clustering algorithm for regression) performs variable selection for regressions with many highly correlated predictors. The OSCAR simultaneously eliminates extraneous variables and performs supervised clustering on the important variables.

Other penalized regression methods have been proposed for grouped predictors (Tibshirani et al., 2005; Yuan and Lin, 2006; Zou and Yuan 2006); however, all of these methods presuppose the grouping structure, e.g., the number of groups or the corresponding sizes. The OSCAR uses a new type of penalty region that is octagonal in shape and requires no initial information regarding the grouping structure. The nature of the penalty region encourages both sparsity and equality of coefficients for correlated predictors having similar relationships with the response. The exact equality of coefficients obtained via this penalty creates grouped predictors as in the supervised clustering techniques. These predictive clusters can then be investigated further to discover what contributes to the group having a similar behavior. Hence, the procedure can also be used as an exploratory tool in a data analysis. Often this structure can be explained by an underlying characteristic, as in the soil example where a group of variables are all related to the abundance of positively charged ions.

The remainder of the article is organized as follows. Section 2 formulates the OSCAR as a constrained least-squares problem and the geometric interpretation of this constraint region is discussed. Computational issues, including choosing the tuning parameters, are discussed in Section 3. Section 4 shows that the OSCAR compares favorably to the existing shrinkage and variable selection techniques in terms of both prediction error and reduced model complexity. Finally, the OSCAR is applied to the soil data in Section 5.

2. The OSCAR

2.1 Formulation

Consider the usual linear regression model with observed data on n observations and p predictor variables. Let $\mathbf{y} = (y_1, \dots, y_n)^T$ be the vector of responses and $\mathbf{x}_j = (x_{1j}, \dots, x_{nj})^T$ denote the j^{th} predictor, $j = 1, \dots, p$. Assume that the response has been centered and each predictor has been standardized so that

$$\sum_{i=1}^n y_i = 0, \quad \sum_{i=1}^n x_{ij} = 0 \quad \text{and} \quad \sum_{i=1}^n x_{ij}^2 = 1$$

for all $j = 1, \dots, p$.

Because the response is centered, the intercept is omitted from the model.

As with previous approaches, the OSCAR is constructed via a constrained least-squares problem. The choice of constraint used here is on a weighted combination of the L_1 norm and a pairwise L_∞ norm for the coefficients. Specifically, the constrained least-squares optimization problem for the OSCAR is given by

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left\| \mathbf{y} - \sum_{j=1}^p \beta_j \mathbf{x}_j \right\|^2$$

subject to

$$\sum_{j=1}^p |\beta_j| + c \sum_{j < k} \max\{|\beta_j|, |\beta_k|\} \leq t, \quad (1)$$

where $c \geq 0$ and $t > 0$ are tuning constants with c controlling the relative weighting of the norms and t controlling the magnitude. The L_1 norm encourages sparseness, while the pairwise L_∞ norm encourages equality of coefficients. Overall, the OSCAR optimization formulation encourages a parsimonious solution in terms of the number of unique nonzero coefficients. Although the correlations between predictors do not directly appear in the penalty term, it is shown both graphically and later in Theorem 1 that the OSCAR implicitly encourages grouping of highly correlated predictors.

While given mathematically by (1), the form of the constrained optimization problem is directly motivated more from the geometric interpretation of the constraint region, rather than from the penalty itself. This geometric interpretation of the constrained least-squares solutions illustrates how this penalty simultaneously encourages sparsity and grouping. Aside from a constant, the contours of the sum-of-squares loss function,

$$(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}^0)^T \mathbf{X}^T \mathbf{X} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}^0), \quad (2)$$

are ellipses centered at the ordinary least squares (OLS) solution, $\hat{\boldsymbol{\beta}}^0$. Because the predictors are standardized, when $p = 2$ the principal axis of the contours are at $\pm 45^\circ$ to the horizontal. As the contours are in terms of $\mathbf{X}^T \mathbf{X}$, as opposed to $(\mathbf{X}^T \mathbf{X})^{-1}$, positive correlation would yield contours that are at -45° whereas negative correlation gives the reverse.

In the (β_1, β_2) plane, intuitively, the solution is the first time that the contours of the sum-of-squares loss function hit the constraint region. The left-hand side panel of Figure 1 depicts the shape of the constraint region for the LASSO and the Elastic Net (Zou and Hastie, 2005), which uses a mixture of L_1 and L_2 penalties. Note that the ridge regression contours (not shown) are circles centered at the origin. As the contours are more likely to hit at a vertex, the nondifferentiability of the LASSO and Elastic Net at the axes encourage sparsity, with the LASSO doing so to a larger degree due to the linear boundary. Meanwhile, if two variables were highly correlated, the Elastic Net would more often include both into the model, as opposed to including only one of the two.

The right-hand side panel of Figure 1 illustrates the constraint region for the OSCAR for various values of the parameter c . From this figure, the reason for the octagonal term in the name is now clear. The shape of the constraint region in two dimensions is exactly an octagon. With vertices on the diagonals along with the axes, the OSCAR encourages both sparsity and equality of coefficients to varying degrees, depending on the strength of correlation, the value of c , and the location of the OLS solution.

Figure 2 shows that with the same OLS solution, grouping is more likely to occur if the predictors are highly correlated.

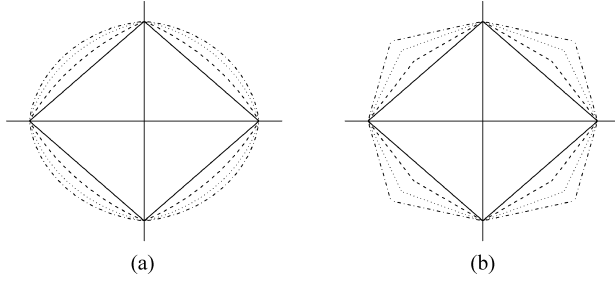


Figure 1. Graphical representation of the constraint region in the (β_1, β_2) plane for the LASSO, Elastic Net, and OSCAR. Note that all are nondifferentiable at the axes. (a) Constraint region for the Lasso (solid line), along with three choices of tuning parameter for the Elastic Net. (b) Constraint region for the OSCAR for four values of c . The solid line represents $c = 0$, the LASSO.

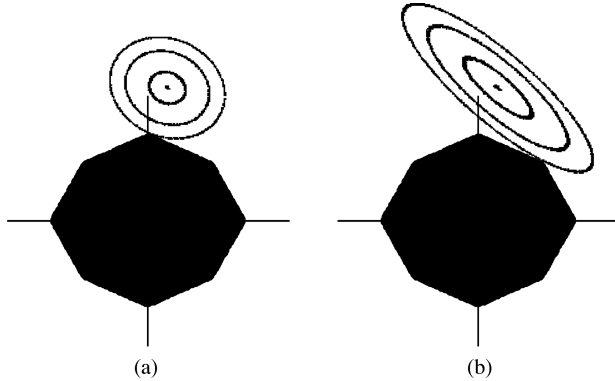


Figure 2. Graphical representation in the (β_1, β_2) plane. The OSCAR solution is the first time the contours of the sum-of-squares function hits the octagonal constraint region. (a) Contours centered at OLS estimate, low correlation ($\rho = 0.15$). Solution occurs at $\hat{\beta}_1 = 0$. (b) Contours centered at OLS estimate, high correlation ($\rho = 0.85$). Solution occurs at $\hat{\beta}_1 = \hat{\beta}_2$.

This implicit relationship to correlation is also quantified later in Theorem 1. Figure 2a shows that if the correlation between predictors is small ($\rho = 0.15$), the sum-of-squares contours first intersect the constraint region on the vertical axis, giving a sparse solution with $\hat{\beta}_1 = 0$. In comparison, the right-hand side panel shows that with the same OLS solution, if the predictors are highly correlated ($\rho = 0.85$), the two coefficients reach equality, and thus the predictors form a group.

Remark. By construction, considering the mirror image, i.e., negative correlation, the coefficients would be set equal in magnitude, differing in sign. This would correspond to using the difference between the two predictors as opposed to the sum, possibly denoting a pair of competing predictors, or that a sign change is appropriate, if applicable.

Note that choosing $c = 0$ in the OSCAR yields the LASSO, which gives only sparsity and no clustering, while letting $c \rightarrow \infty$ gives a square penalty region and only clustering with no variable selection. Varying c changes the angle formed in the

octagon from the extremes of a diamond ($c = 0$), through various degrees of an octagon to its limit as a square, as in two dimensions, $-1/(c+1)$ represents the slope of the line in the first quadrant that intersects the y -axis. In all cases, it remains a convex region.

Remark. Note that the pairwise L_∞ is used instead of the overall L_∞ . Although in two dimensions they accomplish the identical task, their behaviors in $p > 2$ dimensions are quite different. Using an overall L_∞ only allows for the possibility of a single clustered group, which must contain the largest coefficient, as it shrinks from top down. Defining the OSCAR through the pairwise L_∞ allows for multiple groups of varying sizes, as its higher dimensional constraint region has vertices and edges corresponding to each of these more complex possible groupings.

2.2 Exact Grouping Property

The OSCAR formulation as a constrained optimization problem (1) can be written in the penalized form

$$\begin{aligned} \hat{\beta} &= \arg \min_{\beta} \left\| y - \sum_{j=1}^p \beta_j x_j \right\|^2 \\ &+ \lambda \left[\sum_{j=1}^p |\beta_j| + c \sum_{j < k} \max\{|\beta_j|, |\beta_k|\} \right] \\ &= \arg \min_{\beta} \left\| y - \sum_{j=1}^p \beta_j x_j \right\|^2 + \lambda \sum_{j=1}^p \{c(j-1) + 1\} |\beta|_{(j)}, \end{aligned} \quad (3)$$

with $|\beta|_{(1)} \leq |\beta|_{(2)} \leq \dots \leq |\beta|_{(p)}$, and there exists a direct correspondence between λ and the bound t .

An explicit relation between the choice of the constraint bound t and the penalization parameter λ is now given. This allows for computation using an algorithm as discussed in Section 3 derived via the constraint representation, while also considering properties that can be derived via the equivalent penalized representation. Furthermore, a quantification of the exact grouping property of the OSCAR solution in terms of correlation is then given by Theorem 1.

Consider the representation of the OSCAR in terms of the penalized least-squares criterion (3) with penalty parameter λ . Suppose that the set of covariates (x_1, \dots, x_p) are ordered such that their corresponding coefficient estimates satisfy $0 < |\hat{\beta}_1| \leq \dots \leq |\hat{\beta}_Q|$ and $\hat{\beta}_{Q+1} = \dots = \hat{\beta}_p = 0$. Let $0 < \hat{\theta}_1 < \dots < \hat{\theta}_G$ denote the G unique nonzero values of the set of $|\hat{\beta}_j|$, so that $G \leq Q$.

For each $g = 1, \dots, G$, let

$$\mathcal{G}_g = \{j : |\hat{\beta}_j| = \hat{\theta}_g\}$$

denote the set of indices of the covariates that correspond to that value for the absolute coefficient. Now construct the grouped $n \times G$ covariate matrix $\mathbf{X}^* \equiv [\mathbf{x}_1^* \dots \mathbf{x}_G^*]$ with

$$\mathbf{x}_g^* = \sum_{j \in \mathcal{G}_g} \text{sign}(\hat{\beta}_j) \mathbf{x}_j. \quad (4)$$

This transformation amounts to combining the variables with identical magnitudes of the coefficients by a simple (signed)

summation of their values, as in forming a new predictor from the group mean. Form the corresponding summed weights

$$w_g = \sum_{j \in \theta_g} \{c(j-1) + 1\}.$$

The criterion in (3) can be written explicitly in terms of this “active set” of covariates, as

$$\hat{\theta} = \arg \min_{\theta} \left\| \mathbf{y} - \sum_{g=1}^G \theta_g \mathbf{x}_g^* \right\|^2 + \lambda \sum_{g=1}^G w_g \theta_g, \quad (5)$$

with $0 < \theta_1 < \dots < \theta_G$. In a neighborhood of the solution, the ordering, and thus the weights, remain constant and as the criteria are differentiable on the active set, one obtains for each $g = 1, \dots, G$

$$-2\mathbf{x}_g^{*T}(\mathbf{y} - \mathbf{X}^*\hat{\theta}) + \lambda w_g = 0. \quad (6)$$

This vector of score equations corresponds to those in Zou, Hastie, and Tibshirani (2004) and Zou and Hastie (2005) after grouping and absorbing the sign of the coefficient into the covariate.

Equation (6) allows one to obtain the corresponding value of λ for a solution obtained from a given choice of t , i.e., for all values of g , (6) yields

$$\lambda = 2\mathbf{x}_g^{*T}(\mathbf{y} - \mathbf{X}^*\hat{\theta})/w_g. \quad (7)$$

The octagonal shape of the constraint region in Figure 1 graphically depicts the exact grouping property of the OSCAR optimization criterion. The following theorem quantifies this exact grouping property in terms of the correlation between covariates, showing that the equality of two coefficients is easier to obtain as the correlation between the two predictors increases, in that less penalty is needed on the L_∞ norm to do so.

THEOREM 1: Set $\lambda_1 \equiv \lambda$ and $\lambda_2 \equiv c\lambda$ in the Lagrangian formulation given by (3). Given data (\mathbf{y}, \mathbf{X}) with centered response \mathbf{y} and standardized predictors \mathbf{X} , let $\hat{\beta}(\lambda_1, \lambda_2)$ be the OSCAR estimate using the tuning parameters (λ_1, λ_2) . Assume that the predictors are signed so that $\hat{\beta}_i(\lambda_1, \lambda_2) \geq 0$ for all i . Let $\rho_{ij} = \mathbf{x}_i^T \mathbf{x}_j$ be the sample correlation between covariates i and j .

For a given pair of predictors \mathbf{x}_i and \mathbf{x}_j , suppose that both $\hat{\beta}_i(\lambda_1, \lambda_2) > 0$ and $\hat{\beta}_j(\lambda_1, \lambda_2) > 0$ are distinct from the other $\hat{\beta}_k$. Then there exists $\lambda_0 \geq 0$ such that if $\lambda_2 > \lambda_0$ then

$$\hat{\beta}_i(\lambda_1, \lambda_2) = \hat{\beta}_j(\lambda_1, \lambda_2), \text{ for all } \lambda_1 > 0.$$

Furthermore, it must be that

$$\lambda_0 \leq 2\|\mathbf{y}\| \sqrt{2(1 - \rho_{ij})}.$$

The proof of Theorem 1 is based on the score equations in (6), and is given in Web Appendix A.

In the above notation, λ_2 controls the degree of grouping. As λ_2 increases, any given pair of predictors will eventually group. However, the $\sqrt{2(1 - \rho_{ij})}$ term shows that highly correlated predictors are more likely to be grouped. In particular, if two predictors were identical ($\rho = 1$), they will be grouped for any $\lambda_2 > 0$, i.e., any form of the OSCAR penalty other than the special case of the LASSO.

Remark. In Theorem 1, the requirement of the distinctness of $\hat{\beta}_i$ and $\hat{\beta}_j$ is not as restrictive as may first appear. The \mathbf{x}_i and \mathbf{x}_j may themselves already represent grouped covariates as in (4), then ρ_{ij} represents the correlation between the groups.

3. Computation and Crossvalidation

3.1 Computation

A computational algorithm is now discussed to compute the OSCAR estimate for a given set of tuning parameters (t, c) . Write $\beta_j = \beta_j^+ - \beta_j^-$ with both β_j^+ and β_j^- being nonnegative, and only one is nonzero. Then $|\beta_j| = \beta_j^+ + \beta_j^-$. Introduce the additional $p(p-1)/2$ variables η_{jk} for $1 \leq j < k \leq p$, for the pairwise maxima. Then the optimization problem in (1) is equivalent to

$$\begin{aligned} \text{Minimize: } & \frac{1}{2} \left\| \mathbf{y} - \sum_{j=1}^p (\beta_j^+ - \beta_j^-) \mathbf{x}_j \right\|^2 \\ & \text{subject to} \\ & \sum_{j=1}^p (\beta_j^+ + \beta_j^-) + c \sum_{j < k} \eta_{jk} \leq t, \\ & \eta_{jk} \geq \beta_j^+ + \beta_j^-, \eta_{jk} \geq \beta_k^+ + \beta_k^- \quad \text{for each } 1 \leq j < k \leq p, \\ & \beta_j^+ \geq 0, \beta_j^- \geq 0 \quad \text{for all } j = 1, \dots, p, \end{aligned} \quad (8)$$

where the minimization is with respect to the expanded parameter vector (β^+, β^-, η) .

This is now a quadratic programming problem with $(p^2 + 3p)/2$ total parameters and $p^2 + p + 1$ total linear constraints. The constraint matrix is very large, but it is extremely sparse. The optimization has been performed using the quadratic programming algorithm SQOPT (Gill, Murray, and Saunders, 2005), designed specifically for large-scale problems with sparse matrices. Problems with a few hundred predictors are directly computable using this algorithm.

3.2 Choosing the Tuning Parameters

Choosing the tuning parameters (c, t) can be done via minimizing an estimate of the out-of-sample prediction error. If a validation set is available, this can be estimated directly. Lacking a validation set one can use 5- or 10-fold crossvalidation, or a technique such as generalized crossvalidation (GCV), AIC, BIC, or C_p to estimate the prediction error. In using this form of model selection criteria one would need to use the estimated degrees of freedom as in Efron et al. (2004).

For the LASSO, it is known that the number of nonzero coefficients is an unbiased estimate of the degrees of freedom (Efron et al., 2004; Zou et al., 2004). For the fused LASSO, Tibshirani et al. (2005) estimate the degrees of freedom by the number of nonzero distinct blocks of coefficients. Thus, the natural estimate of the degrees of freedom for the OSCAR is the number of distinct nonzero values of $\{|\hat{\beta}_1|, \dots, |\hat{\beta}_p|\}$. This gives a measure of model complexity for the OSCAR in terms of the number of coefficients in the model.

4. Simulation Study

A simulation study was run to examine the performance of the OSCAR under various conditions. Five setups are considered in this simulation. The setups are similar to those used in

both Tibshirani (1996) and Zou and Hastie (2005). In each example, data are simulated from the regression model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim N(0, \sigma^2).$$

For each example, 100 data sets were generated. Each data set consisted of a training set of size n , along with an independent validation set of size n used solely to select the tuning parameters. For each of the 100 data sets, the models were fit on the training data only. For each procedure, the model fit with tuning parameter(s) yielding the lowest prediction error on the validation set was selected as the final model. For these tuning parameters, the estimated coefficients based on the training set are then compared in terms of the mean-squared error (MSE) and the resulting model complexity. For the simulations, the MSE is calculated as in Tibshirani (1996) via

$$\text{MSE} = (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T V (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}), \quad (9)$$

where V is the population covariance matrix for \mathbf{X} , with prediction error given by $\text{MSE} + \sigma^2$.

The five scenarios are given by:

1. In example 1, $n = 20$ and there are $p = 8$ predictors. The true parameters are $\boldsymbol{\beta} = (3, 2, 1.5, 0, 0, 0, 0, 0)^T$ and $\sigma = 3$, with covariance given by $\text{Cov}(\mathbf{x}_i, \mathbf{x}_j) = 0.7^{|i-j|}$. The first three variables are moderately correlated and similar in effect sizes, while the remaining five are unimportant and also somewhat correlated.
2. Example 2 is the same as example one, except that $\boldsymbol{\beta}_j = (3, 0, 0, 1.5, 0, 0, 0, 2)^T$. Now the important variables have little correlation with one another, but they are more correlated with the unimportant predictors.
3. Example 3 is the same as example one, except that $\beta_j = 0.85$ for all j , creating a nonsparse underlying model.
4. In example 4, $n = 100$ and there are $p = 40$ predictors. The true parameters are

$$\boldsymbol{\beta} = (\underbrace{0, \dots, 0}_{10}, \underbrace{2, \dots, 2}_{10}, \underbrace{0, \dots, 0}_{10}, \underbrace{2, \dots, 2}_{10})^T$$

and $\sigma = 15$, with covariance given by $\text{Cov}(\mathbf{x}_i, \mathbf{x}_j) = 0.5$ for $i \neq j$ and $\text{Var}(\mathbf{x}_i) = 1$ for all i .

5. In example 5, $n = 50$ and there are again 40 predictors. The true parameters are

$$\boldsymbol{\beta} = (\underbrace{3, \dots, 3}_{15}, \underbrace{0, \dots, 0}_{25})^T$$

and $\sigma = 15$. The predictors were generated as:

$$\begin{aligned} \mathbf{x}_i &= Z_1 + \epsilon_i^x, & Z_1 &\sim N(0, 1), & i &= 1, \dots, 5 \\ \mathbf{x}_i &= Z_2 + \epsilon_i^x, & Z_2 &\sim N(0, 1), & i &= 6, \dots, 10 \\ \mathbf{x}_i &= Z_3 + \epsilon_i^x, & Z_3 &\sim N(0, 1), & i &= 11, \dots, 15 \\ \mathbf{x}_i &\sim N(0, 1), & i &= 16, \dots, 40, \end{aligned}$$

where ϵ_i^x are independent identically distributed $N(0, 0.16)$, $i = 1, \dots, 15$. In this model the three equally important groups have pairwise correlations $\rho \approx 0.85$, and there are 25 pure noise features.

Table 1 summarizes both the MSE and complexity of the model in terms of the number of unique nonzero coefficients required in the chosen model. In all examples, the OSCAR produces the least complex model by collapsing some of the predictors into groups. Meanwhile, the simulations show that the OSCAR is highly competitive in prediction. Its MSE is either best or second best in all five examples.

Although the values of the coefficients are the same for examples 1 and 2, the OSCAR generally chooses a smaller model for example 1, as can be seen from the number of degrees of freedom in Table 1. This is due to the interplay between the correlation and the values of the coefficients. This is to be expected, as in example 1, variables with similar coefficients are also highly correlated so the grouping mechanism of the OSCAR is more likely to group both the first three coefficients together, as well as group the remaining five unimportant variables together at zero.

The Elastic Net also performs well in terms of prediction error, particularly in cases such as examples 1, 2, and 5 in which there is higher correlation and the true vector is sparse. Particularly in example 5, the Elastic Net's median MSE is lower than the rest, although upon looking at the quantiles, the distribution of MSE in the 100 samples is somewhat similar to the OSCAR. However, the exact grouping effect of the OSCAR allows for the identification of a group structure among the predictors that is not accomplished by the Elastic Net, as seen in the resulting number of coefficients in the model. The loss in prediction error using the OSCAR for this model could come from the large number of unimportant variables combined with the smaller sample size resulting in some of the unimportant variables being smoothed towards the important ones a bit more. In example 3, when all of the predictors are important and equal in effect, the OSCAR and ridge regression perform extremely well in MSE, while the OSCAR also performs grouping. The coefficients for this example were also varied to allow for unequal, but similar effects and the results were similar, thus omitted. Overall, the OSCAR appears to compete well with the existing approaches in terms of MSE in all cases studied, while yielding the additional grouping information to accomplish the supervised clustering task that is not built into the other procedures.

5. Appalachian Mountains Soil Data

The data for this example come from a study of the associations between soil characteristics and rich-cove forest diversity in the Appalachian Mountains of North Carolina. Twenty 500- m^2 plots were surveyed. The outcome is the number of different plant species found within the plot and the 15 soil characteristics used as predictors of forest diversity are listed in Figure 3. The soil measurements for each plot are the average of five equally spaced measurements taken within the plot. The predictors were first standardized before performing the analysis. Because this data set has only $p = 15$ predictors, it allows for an in-depth illustration of the behavior of the OSCAR solution.

Figure 3 shows that there are several highly correlated predictors. The first seven covariates are all related to the abundance of positively charged ions, i.e., cations. Percent base saturation, cation exchange capacity (CEC), and the sum

Table 1

Simulation study. Median MSEs for the simulated examples based on 100 replications with standard errors estimated via the bootstrap in parentheses. The 10th and 90th percentiles of the 100 MSE values are also reported. The median number of unique nonzero coefficients in the model is denoted by Median Df, while the 10th and 90th percentiles of this distribution are also reported.

Example		Med. MSE (Std. Err.)	MSE 10th perc.	MSE 90th perc.	Med. Df	Df 10th perc.	Df 90th perc.
1	Ridge	2.31 (0.18)	0.98	4.25	8	8	8
	Lasso	1.92 (0.16)	0.68	4.02	5	3	8
	Elastic Net	1.64 (0.13)	0.49	3.26	5	3	7.5
	Oscar	1.68 (0.13)	0.52	3.34	4	2	7
2	Ridge	2.94 (0.18)	1.36	4.63	8	8	8
	Lasso	2.72 (0.24)	0.98	5.50	5	3.5	8
	Elastic Net	2.59 (0.21)	0.95	5.45	6	4	8
	Oscar	2.51 (0.22)	0.96	5.06	5	3	8
3	Ridge	1.48 (0.17)	0.56	3.39	8	8	8
	Lasso	2.94 (0.21)	1.39	5.34	6	4	8
	Elastic Net	2.24 (0.17)	1.02	4.05	7	5	8
	Oscar	1.44 (0.19)	0.51	3.61	5	2	7
4	Ridge	27.4 (1.17)	21.2	36.3	40	40	40
	Lasso	45.4 (1.52)	32.0	56.4	21	16	25
	Elastic Net	34.4 (1.72)	24.0	45.3	25	21	28
	Oscar	25.9 (1.26)	19.1	38.1	15	5	19
5	Ridge	70.2 (3.05)	41.8	103.6	40	40	40
	Lasso	64.7 (3.03)	27.6	116.5	12	9	18
	Elastic Net	40.7 (3.40)	17.3	94.2	17	13	25
	Oscar	51.8 (2.92)	14.8	96.3	12	9	18

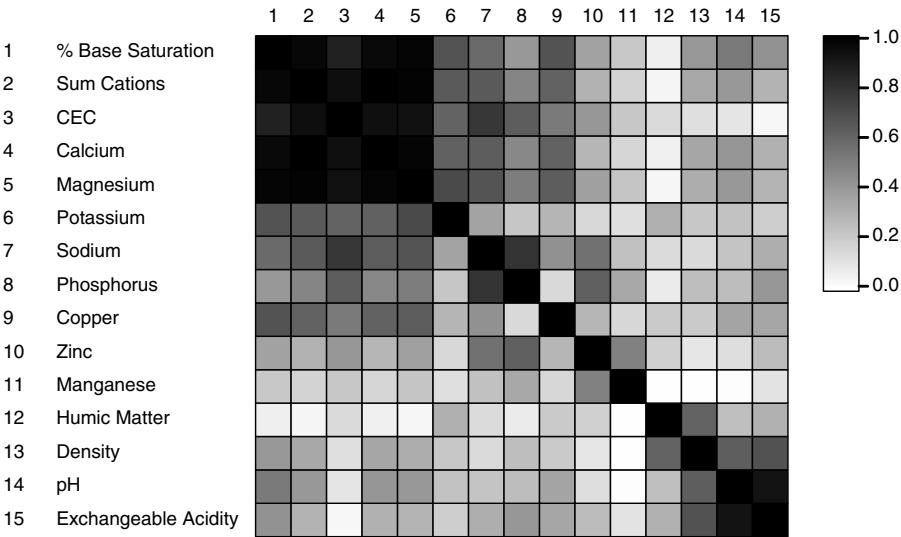


Figure 3. Graphical representation of the correlation matrix of the 15 predictors for the soil data. The magnitude of each pairwise correlation is represented by a block in the grayscale image.

of cations are all summaries of the abundance of cations; calcium, magnesium, potassium, and sodium are all examples of cations. Some of the pairwise absolute correlations between these covariates are as high as 0.95. The correlations involving potassium and sodium are not quite as high as the others. There is also strong correlation between sodium and phosphorus, and between soil pH and exchangeable acidity, two

measures of acidity. Additionally, the design matrix for these predictors is not full rank, as the sum of cations is derived as the sum of the four listed elements. Using fivefold crossvalidation, the best LASSO model includes seven predictors, including two moderately correlated cation covariates: CEC and potassium (Table 2). The LASSO solution paths as a function of s , the proportion of the OLS

Table 2
Estimated coefficients for the soil data example

Variable	OSCAR (5-fold CV)	OSCAR (GCV)	LASSO (5-fold CV)	LASSO (GCV)
% Base saturation	0	-0.073	0	0
Sum cations	-0.178	-0.174	0	0
CEC	-0.178	-0.174	-0.486	0
Calcium	-0.178	-0.174	0	-0.670
Magnesium	0	0	0	0
Potassium	-0.178	-0.174	-0.189	-0.250
Sodium	0	0	0	0
Phosphorus	0.091	0.119	0.067	0.223
Copper	0.237	0.274	0.240	0.400
Zinc	0	0	0	-0.129
Manganese	0.267	0.274	0.293	0.321
Humic matter	-0.541	-0.558	-0.563	-0.660
Density	0	0	0	0
pH	0.145	0.174	0.013	0.225
Exchangeable acidity	0	0	0	0

L_1 norm, for the seven cation-related covariates are plotted in Figure 4a, while the remaining eight are plotted in Figure 4b. As the penalty decreases, the first two cation-related variables to enter the model are CEC and potassium. As the penalty reaches 15% of the OLS norm, CEC abruptly drops out of the model and is replaced by calcium, which is highly correlated with CEC ($\rho = 0.94$). Potassium remains in the model after the addition of calcium, as the correlation between the two is not as extreme ($\rho = 0.62$). Due to the high collinearity, the method for choosing the tuning parameter in the LASSO greatly affects the choice of the model; fivefold crossvalidation includes CEC, whereas GCV instead includes calcium. Clearly, at least one of the highly correlated cation covariates should be included in the model, but the LASSO is unsure about which one.

The fivefold crossvalidation OSCAR solution (Table 2) includes all seven predictors selected by the LASSO along with two additional cation covariates: the sum of cations and calcium. The OSCAR solution groups the four selected cation covariates together, giving a model with six distinct nonzero parameters. The cation covariates are highly correlated and are all associated with the same underlying factor. Therefore, taking their sum as a derived predictor, rather than treating them as separate covariates and arbitrarily choosing a representative, may provide a better measure of the underlying factor and thus a more informative and better predictive model. Note that because the LASSO is a special case of the OSCAR with $c = 0$, the grouped OSCAR solution has a smaller crossvalidation error than the LASSO solution.

The pairs of tuning parameters selected by both fivefold crossvalidation and GCV each have $c = 4$; therefore, Figure 4c and 4d plot the OSCAR solution paths for fixed $c = 4$ as a function of the proportion of the penalty's value at the OLS solution, denoted by s . Tenfold and leave-one-out crossvalidation along with the AIC and BIC criteria were also used and the results were similar. As with the LASSO, CEC is the first cation-related covariate to enter the model as the penalty decreases. However, rather than replacing CEC with calcium as

the penalty reaches 15% of the OLS norm, these parameters are fused, along with the sum of cations and potassium.

Soil pH is also included in the group for the GCV solution. Although pH is not as strongly associated with the cation covariates (Figure 3), it is included in the group chosen by GCV (but not from fivefold crossvalidation) because the magnitude of its parameter estimate at that stage is similar to the magnitude of the cation group's estimate. The OSCAR penalty occasionally results in grouping of weakly correlated covariates that have similar magnitudes, producing a smaller dimensional model. However, by further examining the solution paths in Figure 4c and 4d, it is clear that the more correlated variables tend to remain grouped, whereas others only briefly join the group and are then pulled elsewhere. For example, the GCV solution groups Copper and Manganese, but the solution paths of these two variables' coefficients are only temporarily set equal as they cross. This example shows that more insight regarding the predictor relationships can be uncovered from the solution paths. It is also worth noting that for the eight covariates that are not highly correlated, the OSCAR and LASSO solution paths are similar, as may be expected.

6. Discussion

This article has introduced a new procedure for variable selection in regression while simultaneously performing supervised clustering. The resulting clusters can then be further investigated to determine what relationship among the predictors and response may be responsible for the grouping structure.

The OSCAR penalty can be applied to other optimization criteria in addition to least-squares regression. Generalized linear models with this penalty term on the likelihood are possible via quadratic approximation of the likelihood. Extensions to lifetime data, in which difficulties due to censoring often arise, is another natural next step. In some situations there may be some natural potential groups among the predictors, so one would only include the penalty terms corresponding to predictors among the same group. Examples

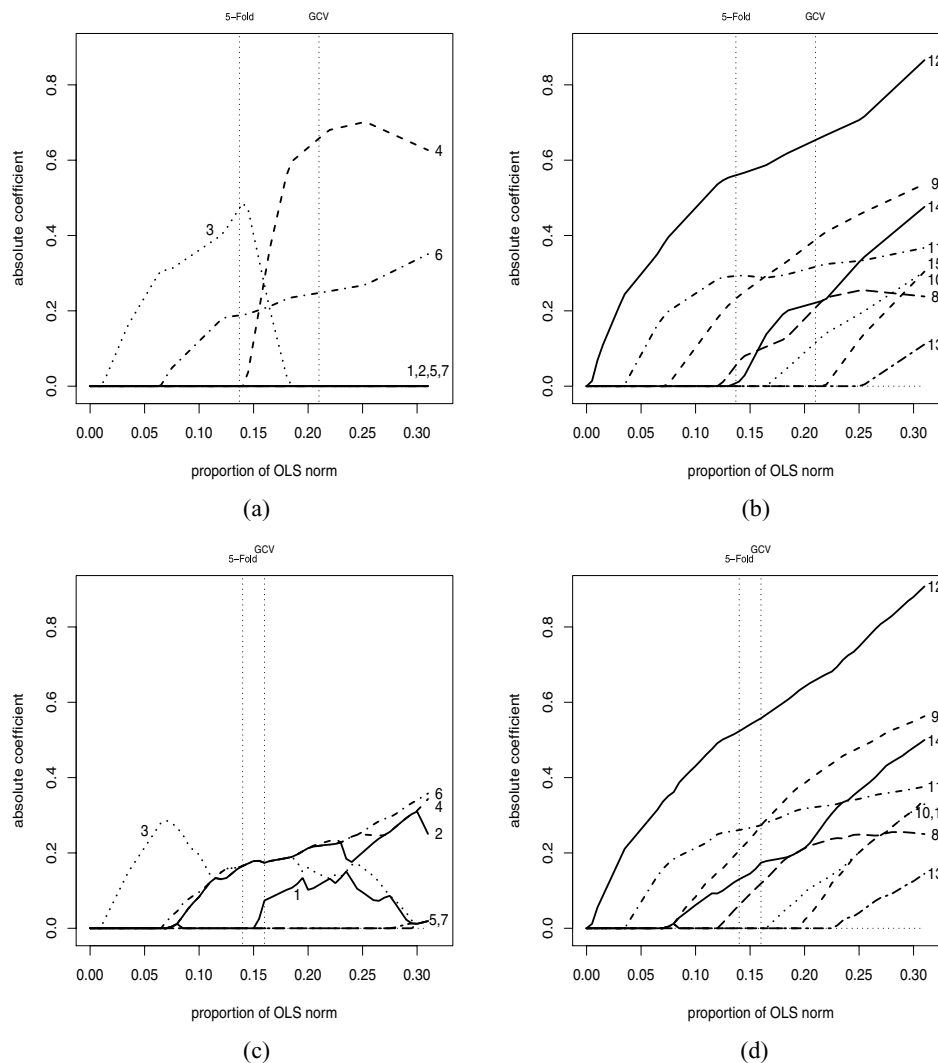


Figure 4. Solution paths for the soil data. Plot of the 15 coefficients as a function of s , the proportion of the penalty evaluated at the OLS solution. The first row uses the fixed value of $c = 0$, the LASSO. The second row uses the value $c = 4$ as chosen by both GCV and fivefold crossvalidation. The vertical lines represent the best models in terms of the GCV and the fivefold crossvalidation criteria for each. (a) LASSO solution paths for the seven cation-related coefficients. (b) LASSO solution paths for the remaining eight coefficients. (c) OSCAR solution paths for the seven cation-related coefficients. (d) OSCAR solution paths for the remaining eight coefficients.

would include ANOVA or nonparametric regression via a set of basis functions.

In the spirit of other penalized regression techniques, the OSCAR solution also has an interpretation as the posterior mode for a particular choice of prior distribution. The OSCAR prior corresponds to a member of the class of multivariate exponential distributions proposed by Marshall and Olkin (1967).

The quadratic programming problem can be large and many standard solvers may have difficulty solving it directly. In the absence of a more efficient solver such as the **SQOPT** algorithm used by the authors, Web Appendix B discusses a sequential method that will often alleviate this problem.

Based on recent results of Rosset and Zhu (2007), for each given c , the solution path for the OSCAR as a function of the bound t , should be piecewise linear. A modification of the least

angle regression (LARS) algorithm that gives the entire solution path for a fixed c , as it does for $c = 0$ would be desirable to dramatically improve computation. However, in addition to adding or removing variables at each step, more possibilities must be considered as variables can group together or split apart as well. Further research into a more efficient computational algorithm is warranted, particularly upon extension to more complicated models.

7. Supplementary Materials

The Web Appendix referenced in Sections 2.2 and 6 is available under the Paper Information link at the *Biometrics* website <http://www.biometrics.tibs.org>. The soil data analyzed in Section 5 and **MATLAB** code to implement the OSCAR procedure for linear regression are also available at the *Biometrics* website.

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