Dimension Reduction via Supervised Clustering of Regression Coefficients: A Review

Suchit Mehrotra
Department of Statistics
North Carolina State University

Abstract

The development and use of dimension reduction methods is prevalent in modern statistical literature. This paper reviews a class of dimension reduction techniques which aim to simultaneously select relevant predictors and find clusters within them which share a common effect on the response. Such methods have been shown to have superior performance relative to OLS estimates and the lasso [Tibshirani, 1996] especially when multicollinearity in the predictors is present. Their applications, which include genetics, epidemiology, and fMRI studies, are also discussed.

1 Introduction

Recent technological advances in computing power and data storage have simplified the collection of vast quantities of data. Modern scientific questions often involve statistical analyses on datasets with a large number of predictors, many of which have no meaningful effect on the response. In numerous situations, an analysis is further complicated by multicollinearity in predictors. An example are microarray studies where interest lies in understanding the relationship between a health outcome and gene expressions; gene expression levels are often highly correlated and the number of genes is substantially larger than the number of samples [Segal et al., 2003].

In a normal linear model, it is well know that ordinary least squares (OLS) is not appropriate in high dimensional situations [Monahan, 2008]. First, if the number of predictors is greater than the number of samples, a unique solution to the OLS optimization problem does not exist. Additionally, if a number of predictors are highly correlated, like in the microarray example, inference in the model is unreliable [Faraway, 2016]. In such situations, it may be reasonable to assume that highly correlated predictors share the same effect on the response, if the correlation is due to the same underlying factor. We can thus reduce the dimension of the problem by summing or averaging groups of highly correlated columns and fitting a linear model with the new set of predictors.
This paper reviews methods which make a slight generalization of this assumption. The methods discussed assume that there exist groups of predictors which have the same effect on the response, but these predictors need not be correlated. Consequently, if we can identify groups with similar effects, we can reduce the dimension of the problem and produce a model with parsimony and superior predictive ability. In essence, this reduces to finding clusters in the regression coefficients in a supervised manner. We focus our attention on the normal linear model, but the reviewed methods can be easily extended to other types of responses. For the rest of this paper let \( y \) be a \( N \times 1 \) vector of responses, \( X \) a \( N \times P \) matrix of covariates, \( \beta \) a \( P \times 1 \) vector of fixed effects, \( e \) a \( N \times 1 \) vector of errors, and

\[
y = X\beta + e, \quad e \sim N(0, \sigma^2 I)
\]

Additionally, assume that the columns of \( X \) are standardized to mean zero and standard deviation one and \( y \) is centered with mean zero.

Many methods have been developed to address the problems posed by OLS in high dimensional settings, with two common approaches being ridge regression and the lasso. Ridge regression [Hoerl and Kennard, 1970] minimizes the residual sum of squares with a restriction on the \( \ell_2 \) norm of the parameter vector \( \beta \). This penalty has the effect of shrinking the elements of \( \beta \) to zero, but it does not produce a parsimonious model. The lasso [Tibshirani, 1996] imposes an \( \ell_1 \) penalty on \( \beta \) which encourages variable selection by shrinking small effects to zero. Because of its variable selection property, the lasso has become the first model of choice in many applications.

However, there exist two common situations in which the lasso fails [Zou and Hastie, 2005]. If the predictor matrix \( X \) has a group of highly correlated columns, the lasso arbitrarily selects only one from the group and sets the other coefficients to zero. Additionally, if \( P > N \), the lasso only selects a maximum of \( N \) variables. These issues are especially relevant in the microarray example, where genes are not only correlated but many more genes than samples might have an effect on the response. To alleviate these issues Zou and Hastie [2005] propose the elastic net, combining the \( \ell_1 \) penalty of the lasso with an \( \ell_2 \) penalty, which estimates similar regression coefficients for groups of correlated variables.

While the elastic net can be effective in practice, it does not directly aim to find clusters in \( \beta \) and many methods have since been developed to improve upon its performance. These extensions aim to solve the supervised clustering problem using three major approaches: two-step methods, discussed in Section 2, penalized regression methods, discussed in Section 3, and mixture models, discussed in Section 4.
2 Two-step approaches

Much of the early work in supervised clustering of regression coefficients focused on two-step procedures with distinct clustering and model fitting steps. Since the correct grouping of predictors with the same effects is not known \textit{a priori}, researchers made the assumption that correlated predictors have correlated effects. Consequently, the work discussed in this section attempts to solve the problem by first finding a clustering of the predictors, averaging the predictors in the same cluster to create a “super-predictor”, and using them to fit a linear model.

\textbf{Hastie et al. 2001} and \textbf{Park et al. 2006} perform a two-step procedure which combines hierarchical clustering with variable selection methods, such as stepwise selection and the lasso. Algorithm 1 details the method used by \textbf{Park et al. 2006}. Two parameters in the algorithm need to be estimated from the data using cross validation: the level at which to cut the tree, $p$, and the tuning parameter for the lasso, $\lambda$.

\begin{algorithm}
\caption{Hierarchical Clustering and Averaging for Regression \cite{Park2006}}
\begin{algorithmic}
\STATE Generate a dendogram by hierarchically clustering the predictors, creating a hierarchy of $P$ possible clusterings.
\FOR{$p = 1$ \TO $P$} 
\STATE Create a new response matrix, $\tilde{X}_p$, by averaging all the clusters at level $p$.
\STATE Regress $y$ on $\tilde{X}_p$ using the lasso, with tuning parameter $\lambda$, to get estimate $\hat{\beta}_{p,\lambda}$
\ENDFOR
\STATE Choose $p$ and $\lambda$ using cross-validation
\end{algorithmic}
\end{algorithm}

Another two-step algorithmic approach is given by \textbf{Jörnsten and Yu 2003}, who use an iterative method to simultaneously cluster genes and classify a response of interest. The first part of their model is a clustering step which uses a Gaussian mixture model and the second averages columns in a cluster to create new predictors for classifying the response. \textbf{Dettling and Bühlmann 2004} propose a similar method with an algorithm which iterates between clustering the predictors into groups and fitting a logistic regression model.

A more recent two-step approach is proposed by \textbf{Bühlmann et al. 2013}, who first cluster the columns of $X$ and then use these groups for parameter estimation via the group lasso \cite{YuanLin2006}.

There are multiple drawbacks to the procedures described above. First, averaging correlated predictors is only a proxy for the supervised clustering of regression coefficients, not a direct solution to the problem. If two correlated predictors have different effects, it is easy to see how the two-step approach can lead to poor estimates. Second, parameter estimation for these methods requires solving a non-convex optimization problem. Hierarchical clustering, used by \textbf{Park et al. 2006}, is performed using heuristic based agglomerative algorithms and always provides a clustering of the data even if none exists \cite{Murphy2012}. Third, two-step procedures do not lend themselves to clear uncertainty quantification. Even if we replace the lasso in
Algorithm [1] with a linear model, standard error estimates given by linear model theory would not account for the uncertainty in the clustering of \( X \).

The penalization based approaches considered in the next section effectively resolve the first two issues. They impose penalties which encourage coefficients to shrink to one another and allow for estimation of \( \beta \) by solving a convex optimization problem.

## 3 Penalization Based Methods

The primary approach for dimension reduction in the frequentist literature is to induce sparsity in \( \beta \) via penalized regression. An estimate for the coefficients is found by solving an optimization problem which minimizes the residual sum of squares along with a penalty on the coefficients. Generally, the loss function can be written in the form of Equation 2 where \( \Omega(\beta) \) is a penalty term used to impose structure on \( \beta \).

\[
\mathcal{L}(\beta, \lambda) = \frac{1}{2}||y - X\beta||_2^2 + \lambda\Omega(\beta) \tag{2}
\]

The ideal penalty to induce sparsity in this context is the \( \ell_0 \) norm, \( \Omega(\beta) = ||\beta||_0 \), which counts the number of non-zero entries in \( \beta \). However, this penalty leads to a NP-Hard optimization problem and is computationally infeasible even for relatively small data sets [She, 2010]. A popular convex relaxation to the \( \ell_0 \) norm is the lasso which uses \( \Omega(\beta) = ||\beta||_1 = \sum_{j=1}^{P} |\beta_j| \) [Tibshirani, 1996].

The lasso’s \( \ell_1 \) penalty can be modified to impose general structural constraints which encompass a wide variety of problems. The modified optimization problem is called the generalized lasso [Tibshirani and Taylor, 2011] and its solution is given by

\[
\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^P} \frac{1}{2}||y - X\beta||_2^2 + \lambda||D\beta||_1 \tag{3}
\]

where \( D \in \mathbb{R}^{M \times P} \) is a prespecified penalty matrix. We will see below that most of the penalization methods discussed can be cast into the generalized lasso framework. This allows for efficient computation of parameter estimates via the use of a path algorithm developed by [Tibshirani and Taylor, 2011].

Before we list specific methods which perform supervised clustering of regression coefficients, it is useful to discuss the general framework for finding clusters via convex penalized regression. This will motivate the types of penalties used in the regression methods below.
3.1 Convex Clustering

Solutions to common clustering algorithms such as $k$-means and hierarchical clustering are found by optimizing a non-convex function. This not only makes the problem computationally intensive, but their solutions can also suffer from instability. Recent advances [Lindsten et al., 2011, Hocking et al., 2011] aim to remedy these issues by using a convex relaxation of the clustering problem. Clusters in the data can be found via penalized regression for a particular choice of the tuning parameter. Given $N$ points, $x_1, \ldots, x_N$ in $\mathbb{R}^m$, they optimize

$$L(U, \lambda, w) = \frac{1}{2} \sum_{i=1}^{N} ||x_i - u_i||_2^2 + \lambda \sum_{i<j} w_{ij} ||u_i - u_j||_p$$

where $\lambda > 0$ is a tuning parameter, $w_{ij}$ is a non-negative weight, $|| \cdot ||_p$ is an arbitrary norm, and $u_i$ is the cluster center for point $x_i$. The penalty on the differences $(u_i - u_j)$ forces the cluster centers towards one another and, as $\lambda \to \infty$, $u_i = u_j$ for all $i \neq j$. A clustering result similar to hierarchical clustering can also be generated by solving Equation 4 at different values of $\lambda$; as $\lambda$ goes from zero to $\infty$ the number of clusters goes from $N$ to 1. Additionally, for given $\lambda$ and $w$, Equation 4 has a unique global minimizer and can be solved with fast iterative algorithms developed by Chi and Lange [2015].

Equation 4 is useful in seeing how penalizing differences in the elements of $\beta$ can promote clustering of regression coefficients. The first use of such penalties was the fused lasso [Tibshirani et al., 2005] which penalizes coefficients of neighbouring covariates. Parameter estimates for the fused lasso are given by:

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2} ||y - X\beta||_2^2 + \lambda_1 ||\beta||_1 + \lambda_2 \sum_{j=2}^{P} |\beta_j - \beta_{j-1}|$$

This approach incorporates variable selection and clustering into the same optimization problem. The first term in the penalty encourages sparsity in the coefficients, while the second encourages sparsity in successive differences. Like with convex clustering, as $\lambda_2 \to \infty$ successive differences in $\beta$ go to zero and $\beta_i = \beta_j$ for all $i \neq j$.

It can easily be seen that the fused lasso problem given by Equation 5 can be cast as a generalized lasso, albeit with two tuning parameters. For example, if $\beta \in \mathbb{R}^3$ the $D$ which makes Equation 5 equivalent to Equation 4 is

$$D_{\lambda_2} = \begin{bmatrix} I \\ \lambda_2 F \end{bmatrix} \text{ where } F = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$$

(6)
Consequently, the fused lasso solution is also given by

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|y - X\beta\|_2^2 + \lambda_1||D\lambda_2\beta||$$

with the matrix $D\lambda_2$ having the form given in (6).

### 3.2 Clustered Lasso

While the fused lasso works for ordered coefficients, it is too restrictive for most applications. This issue is addressed by the clustered lasso, which is again a special case of the generalized lasso [She, 2010]. The clustered lasso estimates are given by:

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|y - X\beta\| + \lambda_1||\beta||_1 + \lambda_2 \sum_{i<j}|\beta_i - \beta_j|$$

While the clustered lasso is a simple combination of the convex clustering penalty with a variable selection penalty, [She, 2010] shows that it is inconsistent for identifying the correct clustering of $\beta$. This issue is due to the use of an $\ell_1$ relaxation, and [She, 2010] proposes a multi-step algorithm, combining data augmentation and adaptive weights, to remedy the issue [Zou, 2006]. Given $\hat{\beta}_a$ and $\hat{\beta}_w$, the new solution is found by solving the following optimization problem:

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|y^* - X^*\beta\|_2^2 + \lambda_1 \sum w_i|\lambda_2\hat{\beta}_w|$$

where $y^* = [y^T, y_a^T]^T$, and $X^* = [X^T, X_a^T]^T$, $X_a = \sqrt{\tau}A(\hat{\beta}_a)$, $y_a = 0$, $w_i = 1/|\lambda_2\hat{\beta}_w|$, and $A(\beta)$ is given by

$$A(\beta) = \begin{cases} I - \beta\beta^T/||\beta||_2^2 & \text{if } \beta \neq 0 \\ I & \text{if } \beta = 0 \end{cases}$$

The problem in Equation (9) is called the data augmented weighted clustered lasso (DAW-CLASSO). [She, 2010] proposes solving the problem multiple times to improve parameter estimates as given in Algorithm (2).

Obvious computational bottlenecks exist in this approach. First, we have to solve multiple problems to get one solution to (9) and repeating these steps is inefficient. Second, the DAW-CLASSO has three tuning parameters, $\tau$, $\lambda_1$, and $\lambda_2$, and a grid search with cross-validation needs to be incorporated to find their optimal values.
Algorithm 2: DAW-CLASSO  \cite{She, 2010}

1 Solve Problem \[8\] Call the estimate $\hat{\beta}_c$
2 repeat
3 Sort $\hat{\beta}_c$ in ascending order
4 Fit the fused lasso \[5\] according the order in Step 3. Label the estimate $\hat{\beta}_f$
5 Substitute $\hat{\beta}_a$ with $\hat{\beta}_c$ and $\hat{\beta}_f$ for $\hat{\beta}_w$
6 Create $y^*$ and $X^*$ and solve \[9\]. Overwrite $\hat{\beta}_c$ with this estimate
7 until desired;

3.3 OSCAR

Another two part penalty which encourages sparsity and clustering in $\beta$ is OSCAR \cite{Bondell and Reich, 2008}. They propose combining an $\ell_1$ penalty with an $\ell_\infty$ penalty, which encourages the absolute value of coefficient pairs to be equal. The solution to their problem is given by:

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2}||y - X\beta||_2^2 + \lambda_1||\beta||_1 + \lambda_2 \sum_{i<j} \max\{|\beta_i|, |\beta_j|\}$$

(11)

While this problem is convex, the penalty on $|\beta|$ increases its computational complexity relative to methods which penalize differences in $\beta$. In their paper, \cite{Bondell and Reich, 2008} solve the problem by expanding $\beta_j$ into $\beta_j^+ - \beta_j^- (\beta_j^+, \beta_j^- \geq 0)$ and introducing auxiliary variables for the pairwise maxima. They estimate $\beta$ using a quadratic program with $(P^2 + 3P)/2$ parameters and $P^2 + P + 1$ linear constraints. \cite{Zhong and Kwok, 2012} solve the problem with an efficient the accelerated projected gradient method but it is not implemented in any statistical software.

However, like with the clustered and fused lasso, OSCAR can be cast as a generalized lasso. Using the identity $\max\{|\beta_j|, |\beta_k|\} = \frac{1}{2}(|\beta_k - \beta_j| + |\beta_j + \beta_k|)$ the penalty in (11) becomes $\lambda_1||\beta||_1 + \frac{\lambda_2}{2} \sum_{i<j} |\beta_i - \beta_j| + \frac{\lambda_2}{2} |\beta_i + \beta_j|$. An appropriate $D_{\lambda_2}$ like in \[6\] can be created for this penalty, and the generalized lasso path algorithm can be used for fixed $\lambda_2$.

3.4 PACS

\cite{Sharma et al., 2013} propose a penalty called pairwise absolute clustering and shrinkage (PACS) to address problems with OSCAR. Like the naive clustered lasso in \[8\], the authors note that OSCAR is not an oracle procedure \cite{Fan and Li, 2001}. As done by \cite{She, 2010} for the clustered lasso, they propose an adaptive weighting scheme and show that PACS is a method with oracle properties. The PACS coefficient estimates
are given by:
\[
\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^P} \frac{1}{2}||y - X\beta|| + \lambda \left\{ \sum_{j=1}^{P} w_j |\beta_j| + \sum_{j<k} w_{jk(-)} |\beta_j - \beta_k| + \sum_{j<k} w_{jk(+)} (|\beta_j + \beta_k|) \right\}
\]

The PACS penalty combines an $\ell_1$ norm to encourage sparsity in the coefficients and penalizes their sum and differences to encourage sparsity in their absolute differences. This effect of PACS is similar to that of OSCAR and, using the identity $\max\{|\beta_j|, |\beta_k|\} = \frac{1}{2}(|\beta_k - \beta_j| + |\beta_j + \beta_k|)$, it can be shown that OSCAR is a special case of PACS.

There are two differentiating factors between OSCAR and PACS. First, PACS incorporates non-negative weights $(w_j, w_{jk(+)}, w_{jk(-)})$ which allow an analyst to incorporate additional prior information into the model. The authors discuss two general methods for choosing weights: data adaptive weights and weights related to the correlation between predictors. Additionally, PACS enjoys computational advantages relative to the penalization approaches mentioned earlier. Like the penalties above, PACS can be recast as a generalized lasso for an appropriate structure matrix $D$. However, unlike the fused lasso, clustered lasso, and OSCAR, the resulting penalty matrix will only have one tuning parameter. This allows the full coefficient path to be estimated by only one run of the algorithm developed by [Tibshirani and Taylor 2011].

3.5 Other Methods

The above list of methods is by no means exhaustive. Many other penalized regression approaches exist, but rely on the assumption that correlated columns have similar effects. For example, [Witten et al. 2014] propose the Cluster Elastic Net, where clusters in $\beta$ are encouraged to form for highly correlated predictors, and groups for the columns of $X$ are learned in a data adaptive fashion. [Li et al. 2018] propose a three-part penalty to estimate coefficients by assuming an underlying graph structure in $X$ and use an estimate of its covariance for adaptive weighting. Their method incorporates many other approaches as special cases and we refer the reader to their paper for details.

3.6 Issues with penalization based approaches

The methods discussed in this section suffer from three major issues. First, regardless of the asymptotic proofs provided by [She 2010] and [Sharma et al. 2013], no method gives an exact clustering of the regression coefficients in finite samples. To estimate a clustering, the above approaches need to be augmented with a procedure such as $k$-means or hierarchical clustering, but choosing the number of clusters remains an unresolved question. Second, none of the methods mentioned above provide clear guidance on uncertainty
quantification for the coefficient estimates. The default choice in most situations would be to use the bootstrap [Efron and Tibshirani, 1994] but it is known to fail for $\ell_1$ penalties [Kyung et al., 2010]. Finally, tuning parameter selection can be a computational bottleneck for the methods discussed; all but PACS have a tuning parameter in the structure matrix, $D$, and finding their optimal values requires the use of a grid search. Resolution of these issues from the frequentist perspective are open problems. Their solutions have the potential for widespread use since frequentist methods tend to be computationally efficient relative to their Bayesian counterparts.

### 3.7 Bayesian corollaries of penalized regression

The issues of uncertainty quantification and tuning parameter selection can be resolved in the Bayesian context, albeit at greater computational cost. All methods discussed in this section have Bayesian analogs for which Gibbs samplers can be used. Such methods would provide an estimate of the posterior distribution for all parameters and uncertainty quantification would include uncertainty regarding the tuning parameter. Additionally, these methods would allow for the use of priors such as the Horseshoe [Carvalho et al., 2010], Horseshoe+ [Bhadra et al., 2017], and Dirichlet-Laplace [Bhattacharya et al., 2015], all of which have superior shrinkage properties relative to the Laplace distribution.

Unfortunately, even Bayesian penalized regression would fail to provide a clustering of the data without using a second step. This issue can be remedied by the use of mixture models as discussed in Section 4.

### 4 Mixture Models

The methods mentioned in the previous sections have been unsatisfactory in a few ways. Two-step processes do not solve the coefficient clustering problem directly while penalization based approaches fail to set coefficients exactly equal to each other in finite samples. Additionally, in the frequentist setup, uncertainty quantification remains an open problem for both approaches. These issues are best resolved in the Bayesian context with the use of mixture distributions as a prior for $\beta$.

In this section we first discuss finite mixture models and how they can be used to find clusters in $\beta$. We then extend this discussion to countably infinite mixture models and the use of Dirichlet Process priors for the regression coefficients.

### 4.1 Finite Mixture Models

Finite mixture models provide a useful framework for clustering a vector of points $\{y_1, \ldots, y_N\}$ [Murphy, 2012]. Assuming we want to partition the data into $K$ underlying groups, we can model the $y_i$ as a mixture
distribution of the form \( f(y_i|K, \pi, \theta) = \sum_{k=1}^{K} \pi_k f_k(y_i|\theta_k) \) where \( \theta = \{\theta_1, \ldots, \theta_k\} \) is a set of parameters which index the \( k \)'th base distribution, \( f_k \), and \( \pi \) is a vector of mixing weights with \( \pi_i \geq 0 \) and \( \sum_i \pi_i = 1 \).

Finite mixture models are commonly given a latent class representation where the elements of a vector, \( c \), are used to encode class membership for the elements of \( y \). Because our end goal is coefficient clustering in normal linear models, assume that each base distribution is normal with varying mean and constant variance. The finite mixture model can be then be written hierarchically as follows:

\[
\begin{align*}
y_i|c_i = k, \theta &\sim \mathcal{N}(\theta_k, \sigma^2) \\
c_i|\pi &\sim \text{Discrete}(\pi_1, \ldots, \pi_K) \\
\pi|\alpha, K &\sim \text{Dirichlet} \left( \frac{\alpha}{K} 1_K \right) \\
\theta_k &\sim G_0
\end{align*}
\]

From the above it can be seen that the mean of each observation, \( \mu_i \), is equal to \( \sum_{k=1}^{K} I(c_i = k) \theta_k \), and that the elements of the mean vector, \( \mu = (\mu_1, \ldots, \mu_N)^T \), can take on only one of \( K \) values. Therefore, we can view \( c \) as a vector of class labels for the elements of \( \mu \) instead of \( y \). Additionally, because \( y|\mu, \sigma^2 \sim \mathcal{N}(I_N \mu, \sigma^2 I_N) \), we can easily modify the hierarchy in (13) to incorporate a covariate matrix \( X \) and parameter vector \( \beta \), as follows:

\[
\begin{align*}
y|\beta, X, \sigma^2 &\sim \mathcal{N}(X\beta, \sigma^2 I) \\
(\forall p \in \{1, \ldots, P\}) \beta_p|c_p, \theta &\sim \sum_{k=1}^{K} I(c_p = k) \theta_k \\
(\forall p \in \{1, \ldots, P\}) c_p|\pi &\sim \text{Discrete}(\pi_1, \ldots, \pi_K) \\
\pi|\alpha &\sim \text{Dirichlet} \left( \frac{\alpha}{K} 1_K \right) \\
(\forall k \in \{1, \ldots, K\}) \theta_k|\gamma &\sim \mathcal{N}(0, \gamma^2)
\end{align*}
\]

Here \( c \) is a \( P \times 1 \) vector which stores class labels for the elements of \( \beta \).

The hierarchy in (14) further implies that \( \beta_p \sim G = \sum_{k=1}^{K} \pi_k \delta_{\theta_k}(\beta_p) \) where \( \delta_{\theta_k}(x) \) is 1 if \( x = \theta_k \) and 0 otherwise. Consequently, each element of \( \beta \) is a finite mixture of \( K \) delta functions, and can only take on one of \( K \) values. If we know \( K \) in advance, estimating \( \theta \) and class memberships, \( c \), provides a solution to the coefficient clustering problem.

Unfortunately, in almost all applications \( K \) is unknown and we need to estimate the number of clusters in \( \beta \). One way to do this is to fit the model in (14) for different values of \( K \) and use a model selection criteria such as cross validation. However, since we are focusing our attention to the Bayesian context, we can put
a prior on the distribution $G$, called a Dirichlet Process, which returns discrete distributions as its samples. The Dirichlet Process is indexed by a concentration parameter, $\alpha$, and a base measure, $G_0$, and its use in the coefficient clustering problem will be our focus for the next three sections.

### 4.2 Dirichlet Processes

The Dirichlet Process (DP) was first investigated by Ferguson [1973] and Antoniak [1974]. Using a stick-breaking construction of the DP, it can be shown that the distribution $G(x) = \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k}(x)$ is a sample from a $DP(\alpha, G_0)$, where $\pi_k = V_k \prod_{l=1}^{k-1} (1 - V_l)$, $V_k \text{iid} \sim \text{Beta}(1, \alpha)$, and $\theta_k \text{iid} \sim G_0$ Sethuraman [1994]. Hence, distributions sampled from the Dirichlet Process are a countably infinite mixture of point masses, which is a generalization of the finite mixture prior for $\beta$ discussed above.

If we use the Dirichlet Process to allow the finite mixture model in (13) to have a variable number of clusters, the resulting model is called a Dirichlet Process mixture model. Computationally efficient methods for estimating such models were developed by Escobar and West [1995], MacEachern and Müller [1998], and Neal [2000]. The model hierarchy is given below:

$$y_i | \mu_i \sim f(\mu_i)$$
$$\mu_i | G \sim G$$
$$G \sim DP(G_0, \alpha)$$

(15)

A key insight into the behaviour of the DP was given by Blackwell et al. [1973] who show that, in exchangeable models, the prior distribution of $\mu_i$ conditional on all other observations is given by

$$\mu_i | \mu_{-i} \sim \frac{1}{N-1+\alpha} \sum_{i \neq j} \delta_{\mu_j}(\mu_i) + \frac{\alpha}{N-1+\alpha} G_0$$

(16)

where $\mu_{-i}$ is the vector $\mu$ without the element $\mu_i$. Neal [2000] gives a similar conditional prior for the class labels, $c$, by viewing the Dirichlet process mixture model as the limit of finite mixture models as $K \to \infty$. By integrating out the mixing parameters $\pi$ he derives the following conditional priors for the elements of $c$

$$P(c_i = k | c_{-i}) = \frac{n_{-i,k}}{N-1+\alpha}$$
$$P(c_i \neq c_j \text{ for all } i \neq j | c_{-i}) = \frac{\alpha}{N-1+\alpha}$$

(17)

where $n_{-i,k}$ is the number of $c_j$, $j \neq i$, that are equal to $k$. These representations allow us to bypass the sampling of mixing weights, $\pi$, and show that the prior conditional probability of an observation being
assigned to an existing cluster is proportional to the number of elements in the cluster.

4.3 Dirichlet Process Priors for Regression

The hierarchy in (14) can be modified to include a Dirichlet Process prior for $\beta$. Nott [2008] explored the estimation and predictive capacity of the DP prior with a normal base measure along with its applications in penalized spline smoothing. The full model hierarchy of his paper is as follows:

$$y|\beta, X, \tau \sim N(X\beta, \tau^{-1}I)$$

$$\forall p \in \{1, \ldots, P\} \beta_p|G \sim G$$

$$G \sim DP(G_0, \alpha)$$

$$G_0|\lambda = N(0, \lambda^{-1})$$

$$\tau \sim \mathcal{G}(a_\tau, b_\tau)$$

$$\lambda \sim \mathcal{G}(a_\lambda, b_\lambda)$$

$$\alpha \sim \mathcal{G}(a_\alpha, b_\alpha)$$

(18)

Nott [2008] derived an efficient Gibbs sampler for the model in (18) by leveraging a latent class representation for group membership. His algorithm iterates between sampling the cluster indicators for the elements of $\beta, c$, and all other model parameters conditioned on the number of clusters in $c, K$. We discuss the salient details of the algorithm below and refer the reader to the original paper for a full derivation.

Conditional on $c$ we need to estimate only $K$ true effects, $\theta$. We can define a $P \times K$ matrix $C$ whose rows are one hot encoded with class membership labels ($C_{pk} = 1$ if $c_p = k$ and 0 otherwise) and see that $y \sim N(XC\theta, \tau^{-1}I_N)$ with $\beta = C\theta$. Since the elements of $\theta$ are samples from $G_0$, it has a $K$ dimensional multivariate normal prior and its update is a simple Bayesian linear regression update with a normal prior.

Updating $c$ is the most computationally intensive step of the Gibbs sampler because its elements have to be updated sequentially. To update the class label for a predictor, $c_p$, we need to calculate posterior probabilities of the predictor belonging to each cluster. Here, the number of clusters is $K + 1$ where $K$ is the number of unique elements in $c_p$. Nott [2008] updates $c_p$ by integrating out the parameter vector $\theta$, which is important for the mixing of the Markov chains, but requires $K + 1$ matrix inversions for each predictor.
The probability that \( c_p = k \) is given by:

\[
P(c_p = k | c_{-i}, \tau, \lambda, \alpha, \theta, X, y) \propto f(y | \tau, \lambda, c', X) P(c_p = k | c_{-i}, \alpha)
\]

\[
f(y | \tau, \lambda, c', X) = \int f(y | \tau, \theta, X, C', \tilde{K}) f(\theta | \lambda, \tilde{K}) d\theta
\]

\[
= \lambda^{\tilde{K}/2} \left( \frac{\lambda}{\tau} \right)^{\tilde{K}/2} |A|^{-1/2} \exp \left\{ -\frac{\tau}{2} \left( y^T y - y^T \tilde{X} A^{-1} \tilde{X}^T y \right) \right\}
\]

where \( A = \tilde{X}^T \tilde{X} + \frac{2}{\lambda} I, \tilde{X} = XC' \), \( c' \) is the vector of class labels with \( c_p = k \), \( \tilde{K} \) is the number of clusters in \( c' \), \( \theta \) is a \( \tilde{K} \times 1 \) vector, and \( P(c_p = k | c_{-i}, \alpha) \) can be calculated by using the formulas in (17). It should be noted that while \( K + 1 \) inverses have to be computed for each predictor, they can be done in parallel to speed up the algorithm.

### 4.4 Point mass + Dirichlet Process Prior

All the penalization methods discussed in Section 3 consist of penalties which aim to perform variable selection and clustering simultaneously. 

Dunson et al. [2008] propose a prior for the same effect, using a mixture of a point mass at zero with a distribution given a DP prior

\[
G = \pi_0 \delta_0 + (1 - \pi_0) G^* \quad G^* \sim DP(\alpha, G_0)
\]

where \( 0 \leq \pi_0 \leq 1 \) is a mixture weight, \( \delta_0 \) is a point mass probability density at 0, and \( DP(\alpha, G_0) \) is a Dirichlet Process prior with precision \( \alpha \) and base measure \( G_0 \). Using the constructive definition of Sethuraman [1994] the prior in (20) is again an infinite mixture of point masses with the first point mass fixed at zero

\[
G = \pi_0 \delta_0 + (1 - \pi_0) \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k} = \sum_{k=0}^{\infty} \tilde{\pi}_k \delta_{\theta_k}
\]

where \( \tilde{\pi}_0 = \pi_0, \tilde{\pi}_k = (1 - \pi_0) \pi_k \) if \( k \geq 1 \), \( \theta_0 = 0 \) and \( \theta_k \overset{iid}{\sim} G_0 \) if \( k \geq 1 \).

Computation for this model is similar to the model discussed in Section 4.3 because the prior in (21) is a clustering prior with the restriction that the first cluster is zero. We can account for this restriction by making a few changes to the Gibbs sampler developed by Nott [2008]. To update \( c \), conditional prior probabilities of the form in (17) need to be determined and the integral in (19) has to be modified by dropping, from \( X \), the columns in the null (zero) cluster. The update of \( \theta \) also relies on dropping the columns in the null cluster because their effects are restricted to be zero; the rest of the update proceeds as before with the smaller
predictor matrix.

If we let \( P_0 \) denote the number of variables which are in the null cluster and \( P_c \) denote the number of variables which are non-zero \( (P = P_0 + P_c) \), we can calculate conditional prior probabilities of the form in (17) by thinking of the prior in two levels: the first being a two component finite mixture model and the second a Dirichlet Process. To begin, we need to determine the prior probabilities of the predictor \( p \) being equal to zero, \( P(c_p = 0|\mathbf{c}_{-p}, \alpha_0) \), where \( [\pi_0, (1 - \pi_0)] \) is given a Dirichlet \( \left( \frac{\alpha_0}{2}, \frac{\alpha_0}{2} \right) \) prior, with \( \pi_0 \sim \text{Unif}(0,1) \) if \( \alpha_0 = 2 \). This is given directly by Neal [2000] to be

\[
\pi^*_0 = \pi(c_p = 0|\mathbf{c}_{-p}, \alpha_0) = \frac{n - p, 0 + \alpha_0/2}{P - 1 + \alpha_0} \tag{22}
\]

Because only a subset of the predictors are non-zero, the Dirichlet Process prior can be thought of as active for only \( P_c \) predictors. Therefore, the probabilities from (22) can be combined with the probabilities from (17) to get the conditional prior for cluster membership

\[
\pi^*_0 = P(c_p = 0|\mathbf{c}_{-p}, \alpha_0) = \frac{n - p, 0 + \alpha_0/2}{P - 1 + \alpha_0}
\]

For \( k \geq 1 \), \( P(c_p = k|\mathbf{c}_{-p}, \alpha) = (1 - \pi^*_0) \left( \frac{n - p, k}{P_c - 1 + \alpha} \right) \)

\[
P(c_p \neq 0 \text{ and } c_p \neq c_j \text{ for all } p \neq j|\mathbf{c}_{-p}, \alpha) = (1 - \pi^*_0) \left( \frac{\alpha}{P_c - 1 + \alpha} \right) \tag{23}
\]

### 4.5 Issues with Mixture Model Approaches

The primary issue with the approaches in this section is their computational complexity. Using Bayesian methods with mixture models as priors for \( \beta \) allows the simultaneous estimation of class membership and uncertainty, but it comes at a cost. While the inversion of multiple matrices in each iteration of the class label update is parallelizable, updating the cluster means, \( \theta \), is not. Therefore, there will always be a step of the Gibbs sampler with computational complexity cubic in the number of clusters. It is reasonable to expect that the number of clusters in \( \beta \) will increase with its size, making such methods computationally infeasible for even moderate \( P \). Possible remedies for this situation could be the use of posterior approximation algorithms such as Variational Bayes [Blei et al., 2017] or Approximate Bayesian Computation [Beaumont, 2010], but their development in the context of Dirichlet Process priors for regression remains an open problem.

### 5 Applications

The methods above have primarily been used to resolve issues with multicollinearity in the predictors. Most early applications were with genetic data, which motivated the development of two-step and most penalized
regression approaches. For example, Hastie et al. [2001] apply a two-step approach to a lymphoma dataset with approximately 3000 gene expression and 36 patients while Zou and Hastie [2005] apply the elastic net to a leukemia dataset with approximately 7000 genes and 70 patients. Another class of problems which can be addressed with such methods arise in epidemiological research, where a large number of correlated exposures are related to a response. For example, MacLehose et al. [2007] apply a Dirichlet Process prior with a point mass at zero to a dataset where the effect of exposure to 18 herbicides on retinal degeneration in approximately 30,000 women was of interest.

A more recent application of these methods has been in the analysis of fMRI data. Technological advances have allowed the collection of large datasets where the columns of $X$ consist of measurements from highly correlated sections of the brain, called voxels. Li et al. [2018] apply their method to an fMRI study where subjects were shown pictures with or without the presence of a human face. Blood-oxygen-level dependent imaging was concurrently conducted to measure activation of neurons, with the goal of classifying the presence of a face in the picture. The final analysis was conducted separately for each individual, where $N = 90$ and $P$ was greater than 5000 for each patient.

6 Conclusion

This paper provides an introduction to many modern dimension reduction techniques which aim to simultaneously select relevant predictors and find groups with the same effect on the response. Such methods were initially developed to address problems which arose in genetic data analysis, but have since been extended to epidemiology and fMRI research. They effectively overcome limitations of popular methods such as the lasso, which often fail to select all predictors related to a response.

In addition to an overview of the methods, a discussion of their respective limitations was also provided. Two-step approaches, while a logical first step to the clustering problem, fail to directly cluster the coefficient vector. Penalized regression approaches, while computationally efficient, are not adequate when an exact clustering of the predictors or uncertainty quantification is required. Finally, while these issues can be effectively resolved in a Bayesian context via the use of Dirichlet Process priors, their use is computationally infeasible for many modern problems, such as the fMRI dataset analyzed by Li et al. [2018].

Ideally, future research will focus on algorithmic developments which allow the application of such models to large datasets, while incorporating parameter estimation, uncertainty quantification, and parameter clustering into one procedure. A fruitful avenue of research could be the development of Variational Bayes algorithms or the exploitation of modern computing technologies, such as GPUs.
References

Charles E. Antoniak. Mixtures of dirichlet processes with applications to bayesian nonparametric problems. *Ann. Statist.*, 2(6):1152–1174, 11 1974.

Mark A Beaumont. Approximate bayesian computation in evolution and ecology. *Annual review of ecology, evolution, and systematics*, 41:379–406, 2010.

Anindya Bhadra, Jyotishka Datta, Nicholas G Polson, Brandon Willard, et al. The horseshoe+ estimator of ultra-sparse signals. *Bayesian Analysis*, 12(4):1105–1131, 2017.

Anirban Bhattacharya, Debdeep Pati, Natesh S Pillai, and David B Dunson. Dirichlet–laplace priors for optimal shrinkage. *Journal of the American Statistical Association*, 110(512):1479–1490, 2015.

David Blackwell, James B MacQueen, et al. Ferguson distributions via pólya urn schemes. *The annals of statistics*, 1(2):353–355, 1973.

David M Blei, Alp Kucukelbir, and Jon D McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017.

Howard D Bondell and Brian J Reich. Simultaneous regression shrinkage, variable selection, and supervised clustering of predictors with oscar. *Biometrics*, 64(1):115–123, 2008.

Peter Bühlmann, Philipp Rütimann, Sara van de Geer, and Cun-Hui Zhang. Correlated variables in regression: clustering and sparse estimation. *Journal of Statistical Planning and Inference*, 143(11):1835–1858, 2013.

Carlos M Carvalho, Nicholas G Polson, and James G Scott. The horseshoe estimator for sparse signals. *Biometrika*, 97(2):465–480, 2010.

Eric C Chi and Kenneth Lange. Splitting methods for convex clustering. *Journal of Computational and Graphical Statistics*, 24(4):994–1013, 2015.

Marcel Dettling and Peter Bühlmann. Finding predictive gene groups from microarray data. *Journal of Multivariate Analysis*, 90(1):106 – 131, 2004. Special Issue on Multivariate Methods in Genomic Data Analysis.

David B Dunson, Amy H Herring, and Stephanie M Engel. Bayesian selection and clustering of polymorphisms in functionally related genes. *Journal of the American Statistical Association*, 103(482):534–546, 2008.
Bradley Efron and Robert J Tibshirani. An introduction to the bootstrap. CRC press, 1994.

Michael D Escobar and Mike West. Bayesian density estimation and inference using mixtures. Journal of the american statistical association, 90(430):577–588, 1995.

Jianqing Fan and Runze Li. Variable selection via nonconcave penalized likelihood and its oracle properties. Journal of the American statistical Association, 96(456):1348–1360, 2001.

Julian J Faraway. Linear models with R. Chapman and Hall/CRC, 2016.

Thomas S. Ferguson. A bayesian analysis of some nonparametric problems. Ann. Statist., 1(2):209–230, 03 1973.

Trevor Hastie, Robert Tibshirani, David Botstein, and Patrick Brown. Supervised harvesting of expression trees. Genome Biology, 2(1):research0003–1, 2001.

Toby Dylan Hocking, Armand Joulin, Francis Bach, and Jean-Philippe Vert. Clusterpath an algorithm for clustering using convex fusion penalties. In 28th international conference on machine learning, page 1, 2011.

Arthur E Hoerl and Robert W Kennard. Ridge regression: Biased estimation for nonorthogonal problems. Technometrics, 12(1):55–67, 1970.

Rebecka Jörnsten and Bin Yu. Simultaneous gene clustering and subset selection for sample classification via mdl. Bioinformatics, 19(9):1100–1109, 2003.

Minjung Kyung, Jeff Gill, Malay Ghosh, and George Casella. Penalized regression, standard errors, and bayesian lassos. Bayesian Anal., 5(2):369–411, 06 2010. doi: 10.1214/10-BA607. URL https://doi.org/10.1214/10-BA607.

Yuan Li, Garvesh Raskutti, and Rebecca Willett. Graph-based regularization for regression problems with highly-correlated designs. arXiv preprint arXiv:1803.07658, 2018.

Fredrik Lindsten, Henrik Ohlsson, and Lemnart Ljung. Just relax and come clustering!: A convexification of k-means clustering. Linköping University Electronic Press, 2011.

Steven N MacEachern and Peter Müller. Estimating mixture of dirichlet process models. Journal of Computational and Graphical Statistics, 7(2):223–238, 1998.

Richard F MacLehose, David B Dunson, Amy H Herring, and Jane A Hoppin. Bayesian methods for highly correlated exposure data. Epidemiology, pages 199–207, 2007.
John F Monahan. *A primer on linear models*. CRC Press, 2008.

Kevin P Murphy. *Machine Learning: A Probabilistic Perspective*. MIT Press, 2012.

Radford M Neal. Markov chain sampling methods for dirichlet process mixture models. *Journal of computational and graphical statistics*, 9(2):249–265, 2000.

David J Nott. Predictive performance of dirichlet process shrinkage methods in linear regression. *Computational Statistics & Data Analysis*, 52(7):3658–3669, 2008.

Mee Young Park, Trevor Hastie, and Robert Tibshirani. Averaged gene expressions for regression. *Biostatistics*, 8(2):212–227, 2006.

Mark R Segal, Kam D Dahlquist, and R Conklin. Regression approaches for microarray data analysis. *Journal of Computational Biology*, 10(6):961–980, 2003.

Jayaram Sethuraman. A constructive definition of dirichlet priors. *Statistica sinica*, pages 639–650, 1994.

Dhruv B. Sharma, Howard D. Bondell, and Hao Helen Zhang. Consistent group identification and variable selection in regression with correlated predictors. *Journal of Computational and Graphical Statistics*, 22(2):319–340, 2013.

Yiyuan She. Sparse regression with exact clustering. *Electronic Journal of Statistics*, 4:1055–1096, 2010.

Robert Tibshirani. Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 267–288, 1996.

Robert Tibshirani, Michael Saunders, Saharon Rosset, Ji Zhu, and Keith Knight. Sparsity and smoothness via the fused lasso. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 67(1):91–108, 2005.

Ryan J. Tibshirani and Jonathan Taylor. The solution path of the generalized lasso. *Ann. Statist.*, 39(3):1335–1371, 06 2011. doi: 10.1214/11-AOS878. URL https://doi.org/10.1214/11-AOS878

Daniela M Witten, Ali Shojaie, and Fan Zhang. The cluster elastic net for high-dimensional regression with unknown variable grouping. *Technometrics*, 56(1):112–122, 2014.

Ming Yuan and Yi Lin. Model selection and estimation in regression with grouped variables. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(1):49–67, 2006.

Leon Wenliang Zhong and James T Kwok. Efficient sparse modeling with automatic feature grouping. *IEEE transactions on neural networks and learning systems*, 23(9):1436–1447, 2012.
Hui Zou. The adaptive lasso and its oracle properties. *Journal of the American statistical association*, 101(476):1418–1429, 2006.

Hui Zou and Trevor Hastie. Regularization and variable selection via the elastic net. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 67(2):301–320, 2005.