Weighted envelope estimation to handle variability in model selection

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Abstract

Envelope methodology can provide substantial efficiency gains in multivariate statistical problems, but in some applications the estimation of the envelope dimension can induce selection volatility that may mitigate those gains. Current envelope methodology does not account for the added variance that can result from this selection. In this article, we circumvent dimension selection volatility through the development of a weighted envelope estimator. Theoretical justification is given for our estimator and validity of the residual bootstrap for estimating its asymptotic variance is established. A simulation study and an analysis on a real data set illustrate the utility of our weighted envelope estimator.

Keywords: Dimension Reduction; Envelope Models; Model Selection; Residual Bootstrap; Variance Reduction.

1 Introduction

Envelope methodology was developed originally in the context of the multivariate linear regression model (Cook, et al., 2010),

\[ Y = \alpha + \beta X + \varepsilon, \]

where \( \alpha \in \mathbb{R}^r, \beta \in \mathbb{R}^{r \times p}, \) the random response vector \( Y \in \mathbb{R}^r, \) the fixed predictor vector \( X \in \mathbb{R}^p \) is centered to have mean zero, and the error vector \( \varepsilon \sim N(0, \Sigma). \) Estimation is assumed to be based on \( n \) independent samples from model (1) where \( n > p. \) It was shown by Cook, et al. (2010) that the envelope estimator of the unknown coefficient matrix \( \beta \) in (1) has the potential to yield massive efficiency gains relative to the maximum likelihood estimator of \( \beta. \) These efficiency gains can arise when the dimension \( u \) of the envelope space, defined in the next section, is less than \( r. \) In most practical applications, \( u \) is unknown and has to be estimated. This estimation can be problematic since the estimated variance of the envelope estimator is typically calculated conditional on the estimated dimension \( \hat{u}. \) Variation associated with model selection is therefore not considered in the current envelope paradigm.

In this article, we propose a weighted envelope estimator of \( \beta \) that smooths out model selection volatility. The weighting is across all possible envelope models under (1). The weights corresponding to each envelope estimator are functions of the Bayesian Information Criterion (BIC) value corresponding to that particular envelope model.
Weighting in this manner is similar to the model averaging techniques discussed by Buckland, et al. (1997) and Burnham and Anderson (2004) who provided a philosophical justification for the use of such weighted estimators without giving any theoretical properties. Hjort and Claeskens (2003) and Liang, et al. (2011) built on the philosophical justification for weighted estimators by deriving their asymptotic properties. Claeskens and Hjort (2008) summarized extensions and applications of the theory of weighted estimators. However, these extensions do not include bootstrap techniques and do not encompass the framework of envelope models. Envelope models fit at dimensions greater than or equal to \( u \) are all true non-nested data generating models and are ordered in preference from dimension \( u \) to \( r \). This context seems novel and is outside of the framework of Claeskens and Hjort (2008).

2 The Envelope Model

The original motivation for envelope methodology came from the observation that, in the multivariate regression model \( \Pi \), some linear combinations of \( Y \) may have a distribution that does not depend on \( X \), while other linear combinations of \( Y \) do depend on \( X \). The envelope model separates out these immaterial and material parts of \( Y \), and thereby allows for efficiency gains (Cook, et al., 2010; Su and Cook, 2011).

More carefully, suppose that we can find a subspace \( S \subseteq \mathbb{R}^r \) so that

\[
Q_S Y \sim P_S Y \ | \ X, \quad \text{and} \quad Q_S Y \ | \ X = x_1 \sim Q_S Y \ | \ X = x_2, \quad \text{for all} \quad x_1, x_2,
\]

where \( \sim \) means identically distributed, \( P_S \) projects onto the subspace indicated by its argument and \( Q = I_r - P \).

For any \( S \) with the properties \( \Pi \), \( P_S Y \) carries all of the material information and perhaps some of the immaterial information, while \( Q_S \) contains just immaterial information. Let \( B = \text{span}(\beta) \) and \( d = \text{dim}(B) \) so that \( 0 < d \leq \min(p, r) \). Then \( \Pi \) holds if and only if \( B \subseteq S \) and \( \Sigma = \Sigma_S + \Sigma_S^\perp \), where \( \Sigma_S = \text{var}(P_S Y) \) and \( \Sigma_S^\perp = \text{var}(Q_S Y) \).

The envelope is defined as the intersection of all subspaces \( S \) that satisfy \( \Pi \) and is denoted by \( E_S(B) \) with dimension \( u = \text{dim} \{ E_S(B) \} \) satisfying \( 0 < d \leq u \leq r \).

The envelope model can be represented in terms of coordinates by parameterizing model \( \Pi \) to incorporate conditions \( \Pi \). Define \( \Gamma \in \mathbb{R}^{r \times u} \) to be a semi-orthogonal basis matrix for \( E_S(B) \) and let \( (\Gamma, \Gamma_u) \in \mathbb{R}^{r \times r} \) be an orthogonal matrix. Then the envelope model with respect to model \( \Pi \) is parameterized as

\[
Y = \alpha + \Gamma \eta X + \epsilon, \quad \epsilon \sim N(0, \Sigma),
\]

where \( \Sigma = \Gamma \Omega \Gamma^T + \Gamma \Omega o \Gamma^T, \ \Omega \in \mathbb{R}^{u \times u} \) and \( \Omega_o \in \mathbb{R}^{(r-u) \times (r-u)} \) are positive definite, and \( \eta \in \mathbb{R}^{u \times p} \) is \( \beta = \Gamma \eta \) in the coordinates of \( \Gamma \). We see from \( \Pi \), that \( E_S(B) \) links the mean and covariance structures of the regression problem and it is this link that provides the efficiency gains. The gains can be massive when the immaterial information is large relative to the material information; for instance, when \( \| \Omega \| \ll \| \Omega_o \| \), where \( \| \cdot \| \) is a matrix norm (Cook, et al., 2010). An illuminating description and explanation of how an envelope increases efficiency in multivariate linear regression problems was given by Su and Cook (2011, pgs. 134–135). Cook and Zhang (2013) provided a more general framework for envelope methodology, which requires only a \( \sqrt{n} \)-consistent estimator \( \hat{\theta} \) of an unknown parameter \( \theta \) and a \( \sqrt{n} \)-consistent estimator of its asymptotic variability. Cook, et al. (2013) showed that partial least squares gives a moment-based envelope estimator that is \( \sqrt{n} \)-consistent. As partial least squares is widely
used in chemometrics and elsewhere, the Cook, et al. (2013) finding indicates that envelope methodology is also widely applicable.

Candidate envelope estimators of $\beta$ at dimension $j$, denoted $\hat{\beta}_j$, are found via maximum likelihood estimation of model (3) with $\hat{\beta}_j = \hat{\Gamma}\hat{\eta}$. An estimator of $u$ is found by using a model selection criterion such as BIC, Akaike Information Criterion (AIC), likelihood ratio tests, or cross-validation. The estimated dimension $\hat{u}$ obtained from any one of these selection criteria is a variable quantity dependent on the observed data. Current envelope methodology does not address this extra variability. In the next two sections, we develop properties of a weighted estimator that takes this extra variability into account.

3 BIC Weighted Estimators

The weighted estimator that we consider is of the form

$$\hat{\beta}_w = \sum_{j=1}^{r} w_j \hat{\beta}_j,$$  \hspace{1cm} (4)

where $\sum_{j=1}^{r} w_j = 1$ and $w_j \geq 0$, for $j = 1, ..., r$. The weights $w_j$ depend on the BIC values for all of the candidate envelope models under consideration. Let the BIC value for the envelope model with dimension $j$ be denoted by $b_j = -2\ell(\hat{\beta}_j) + k(j) \log(n)$, where $\ell(\hat{\beta}_j)$ is the log likelihood evaluated at the envelope estimator $\hat{\beta}_j$ and $k(j) = r + p_j + r(r + 1)/2$ is the number of parameters of the envelope model of dimension $j$. The weight for envelope model $j$ is constructed as

$$w_j = \frac{\exp(-b_j)}{\sum_{k=1}^{r} \exp(-b_k)}.$$  \hspace{1cm} (5)

It follows from arguments in the Supplement that $\hat{\beta}_w$ is a $\sqrt{n}$-consistent estimator of $\beta$, but assessing the variance of $\hat{\beta}_w$ is not so straightforward. In the next section, we show that the residual bootstrap provides a consistent estimator of $\text{var}(\hat{\beta}_u)$. We use BIC in (5) because, in ours and others’ experiences, BIC performs well when selecting the dimension of an envelope model. AIC tends to overselect the true dimension of an envelope model, likelihood ratio testing is inconsistent, and cross-validation is primarily used in prediction problems. We do not claim that BIC is optimal in this application.

4 Bootstrap for $\hat{\beta}_w$

The envelope estimator $\hat{\beta}_u$ at the true dimension $u$ is $\sqrt{n}$-consistent and asymptotically normal (Cook, et al., 2010; Cook and Zhang, 2015). The residual bootstrap used to estimate the variability of $\hat{\beta}_u$ uses the starred responses,

$$Y^* = X\hat{\beta}_u^T + \varepsilon^*,$$  \hspace{1cm} (6)

to obtain $\hat{\beta}_u^*$, where $X \in \mathbb{R}^{n \times p}$ is the fixed design matrix with rows $X_i^T$ and the rows of $\varepsilon^* \in \mathbb{R}^{n \times r}$ are the realizations of $n$ resamples of the residuals from the ordinary least squares fit of (1). This process is performed a total of $B$ times with a new $\hat{\beta}_u^*$ computed from (6) at each iteration. The setup in Andrews (2002, Section 2, pgs. 122-124 and Theorem 2) confirms that the sample variance of the $\hat{\beta}_u^*$s provides a $\sqrt{n}$-consistent estimator of the
asymptotic variability of \( \hat{\beta}_u \). The problem with this approach, as it currently stands, is that \( u \) is unknown. The current implementation of the residual bootstrap implicitly assumes that \( \hat{u} = u. \) Therefore, variability introduced by model selection uncertainty is ignored. This issue is resolved by using \( \hat{\beta}_w \) in place of \( \hat{\beta}_u \) in (6). The next theorem formalizes our asymptotic justification for the use of the weighted envelope estimator \( \hat{\beta}_w \) in practical problems. Its proof is given in the Supplement.

**Theorem 1.** Assume regression model (1) and suppose that an envelope subspace of dimension \( u = 1, \ldots, r \) exists. Assume that \( \Sigma_X = n^{-1}X^T X \to \Sigma_X > 0. \) Let \( \hat{\beta}_w \) be the weighted envelope estimator of \( \beta \) defined in (4) and let \( \hat{\beta}^*_w \) be the weighted envelope estimator of \( \beta \) obtained from resampled data. Then, as \( n \) tends to \( \infty \),

\[
\sqrt{n} \left\{ \text{vec}(\hat{\beta}^*_w) - \text{vec}(\hat{\beta}_w) \right\} = \sqrt{n} \left\{ \text{vec}(\hat{\beta}^*_w) - \text{vec}(\hat{\beta}_u) \right\} \\
+ O_p \left\{ n^{1/2-p} \right\} + 2(u-1)O_p(1)\sqrt{ne^{-n|O_p(1)|}}. \tag{7}
\]

Theorem 1 shows the utility of the weighted envelope estimator \( \hat{\beta}_w \). In (7), we see that the asymptotic distribution of the residual bootstrap at \( \hat{\beta}_w \) is the same as the asymptotic distribution of the residual bootstrap at \( \hat{\beta}_u \). The difference between the two bootstrap procedures is that the bootstrap given in Theorem 1 does not require the conditioning on \( \hat{u} \) as a prerequisite for its implementation.

The orders in (7) result from model selection variability that arises from four sources. The \( O_p \left\{ n^{1/2-p} \right\} \) term corresponds to the rate at which \( \sqrt{nw_j} \) and \( \sqrt{nw_j^*} \) vanish for \( j = u + 1, \ldots, r \). This rate is a cost of over estimation of the envelope space. It decreases quite fast, particularly when \( p \) is not small, because models with \( j > u \) are true and thus have no systematic bias due to choosing the wrong dimension.

The \( 2(u-1)\sqrt{ne^{-n|O_p(1)|}} \) term corresponds to the rate at which \( \sqrt{nw_j} \) and \( \sqrt{nw_j^*} \) vanish for \( j = 1, \ldots, u - 1 \). This rate arises from under estimating the envelope space and it is affected by systematic bias arising from choosing the wrong dimension. To gain intuition about this rate, let \( B_j = \left( G_o^T \Sigma G_o \right)^{-1/2} G_o^T \beta \Sigma X_j^{1/2} \), where \( G_o \in \mathbb{R}^{rx(r-j)} \) is the population basis matrix for the complement of the envelope space of dimension \( j \). This quantity is a standardized version of \( G_o^T \beta \) that reflects bias, since \( G_o^T \beta \neq 0 \) when \( j < u \), but \( G_o^T \beta = 0 \) when \( j \geq u \). Let \( \hat{B}_{j,n} \) denote the \( \sqrt{n} \)-consistent estimator of \( B_j \) obtained by plugging in the sample version of \( \Sigma_X \) and the estimators of \( G_o, \Sigma \) and \( \beta \) that arise by maximizing the likelihood with dimension \( j < u \). Then the \( -n \mid O_p(1) \mid \) term appearing in the exponent of \( 2(u-1)\sqrt{ne^{-n|O_p(1)|}} \) is the rate at which \( -n \log(||I_p + B_{j,n}^T B_{j,n}||) \) approaches \( -\infty \). Additionally, this term is 0 when \( u = 1 \). That arises because we consider only regressions in which \( \beta \neq 0 \) and thus \( u \geq 1 \). When \( u = 1 \) under estimation is not possible in our context and thus \( 2(u-1)\sqrt{ne^{-n|O_p(1)|}} \) vanishes.

The weights in (5) differ from those mentioned in Kass and Raftery (1995) and Tsague (2014). These weights are of the form

\[
\tilde{w}_j = \frac{\exp(-b_j/2)}{\sum_{k=1}^r \exp(-b_k/2)}, \tag{8}
\]

and they correspond to an approximation of the posterior probability for model \( j \) given the observed data under the prior that places equal weight for all candidate models. Weights of the form (8) do not have the same asymptotic properties as the weights given by (5). When \( p = 1 \), the term \( \sqrt{nw_{j+u+1}} \) defined by (8) does not vanish as \( n \to \infty \). We therefore would not have the same asymptotic result given by (7) in Theorem 1. Instead, there
would be non-zero weight placed on the envelope model with dimension $j = u + 1$ asymptotically. This weighting scheme would therefore lead to higher estimated variability than is necessary in practice. However, this issue is no longer problematic when $p > 1$. When $p > 1$ and weights \( w \) are used, the $O_p \{ n^{(1/2-p)} \}$ term in \( T \) becomes $O_p \{ n^{(1-p)/2} \}$, resulting in a slower rate of convergence.

Constructing $\hat{\beta}_w$ with respect to BIC may not be the only weighting scheme that satisfies

$$\sqrt{n} \left\{ \text{vec}(\hat{\beta}_w) - \text{vec}(\hat{\beta}_w) \right\} = \sqrt{n} \left\{ \text{vec}(\hat{\beta}_w) - \text{vec}(\hat{\beta}_w) \right\} + O_p \{ f(p, n) \}$$

where $f(p, n)$ is a function that depends on how the weights are constructed. Any weighting scheme such that, for all $j \neq u$,

$$\sqrt{n} \left\{ \text{vec}(\hat{\beta}_w) - \text{vec}(\hat{\beta}_w) \right\} \rightarrow 0$$

as $n \rightarrow \infty$ satisfies \(9\). Weighting schemes that violate \(10\) will not result in a bootstrap that is consistent.

Similar weights with AIC in place of BIC do not satisfy \(10\). Interchanging BIC with AIC in the proof of Theorem \(1\) produces weights of the form $w_j = O_p(1) \, e^{2(1-k(u)-k(j))}$ for all $j = u + 1, \ldots, r$ which do not vanish as $n \rightarrow \infty$.

5 Examples

We now provide three examples which show the utility of Theorem \(1\). The first two are simulated examples in which we know $\beta$, $\Sigma$, $u$, and $P_{\mathcal{E}_X}(\mathcal{B})$. The third is based on real data.

5.1 Simulated examples

Example 1: For this example we create a setting in which $Y \in \mathbb{R}^3$ is generated according to the model

$$Y_i = \beta X_i + \varepsilon_i, \quad \varepsilon_i \sim \text{iid } N(0, \Sigma),$$

\((i = 1, \ldots, n)\), where $X_i \in \mathbb{R}^2$ is a continuous predictor with entries generated independently from a normal distribution with mean 4 and variance 1. The covariance matrix $\Sigma$ was generated using three orthonormal vectors and has eigenvalues of 50, 10, and 0.01. The matrix $\beta \in \mathbb{R}^{3 \times 2}$ is an element in the space spanned by the second and third eigenvectors of $\Sigma$. We know that the dimension of $\mathcal{E}_X(\mathcal{B})$ is $u = 2$.

| $n$ | 50  | 100 | 500 | 2000 |
|-----|-----|-----|-----|------|
| $\| \text{vec}(\hat{\beta}_u) - \text{vec}(\hat{\beta}_{u+2}) \|$ | 2.3 | 0.16 | 0.0 | 0    |
| $\| \text{vec}(\hat{\beta}_{u+2}) - \text{vec}(\hat{\beta}_{u+2}) \|$ | 0.18 | 0.012 | 0.021 | 0.0051 |

Table 1: Comparison of $\hat{\beta}_u$ and $\hat{\beta}_{u+2}$. The first row is the Euclidean difference between $\text{vec}(\hat{\beta}_u)$ and $\text{vec}(\hat{\beta}_{u+2})$ from the original dataset. The second row is the spectral norm of the estimated variance of the difference of all bootstrap realizations of $\hat{\beta}_u$ and $\hat{\beta}_{u+2}$ with bootstrap sample size $B = n$. 

5
Four datasets were simulated under model (11) at different sample sizes. The multivariate residual bootstrap was used to compare the weighted envelope estimator $\hat{\beta}_w$ with the oracle envelope estimator $\hat{\beta}_u$ across the simulated datasets. In Table 1 we see that the Euclidean difference of $\text{vec}(\hat{\beta}_u)$ and $\text{vec}(\hat{\beta}_w)$ shrinks as $n$ increases, and that the spectral norm of the variance of differences also shrinks as $n$ increases. Taken together, these findings support the conclusions of Theorem 1.

**Example 2:** For this example we illustrate the effect that $p$ has on the performance of the weighted envelope estimator. We generated data according to model (11) with $Y \in \mathbb{R}^5$. In this example $u = 1$ and $\Sigma$ is compound symmetric with diagonal entries set to 1 and off-diagonal entries set to 0.5, $\beta = 1_r c_p^{T}$, where $1_r$ is the $r \times 1$ vector of ones, and $c_p$ is a $p \times 1$ vector where every entry is 10. We generate the predictors according to $X \sim N(0, I_p)$, where $I_p$ is the $p$-dimensional identity matrix. We set $n = 250$.

We then perform a residual bootstrap with sample size $B = 250$ and, for each $p$ considered, we report the number of times each dimension was selected by BIC, denoted by $n(\hat{u})$. From Table 2 we see that the distribution of $\hat{u}$, across the $B$ resamples, approaches a point mass at the truth as $p$ increases with $u$ fixed. This implies that our bootstrap procedure improves as $p$ increases with $u$ fixed, as indicated by Theorem 1.

| $p$ | $n(\hat{u} = 1)$ | $n(\hat{u} = 2)$ | $n(\hat{u} = 3)$ |
|-----|------------------|------------------|------------------|
| 2   | 128              | 111              | 11               |
| 5   | 214              | 34               | 2                |
| 10  | 249              | 1                | 0                |
| 25  | 250              | 0                | 0                |

Table 2: The bootstrap distribution of $\hat{u}$ as $p$ increases, where $\hat{u}$ is selected by BIC and $n(\hat{u} = j)$ is the number of times BIC selected envelope dimension $j$.

### 5.2 Cattle data

The data in this example, analyzed in [Kenward (1987)](https://doi.org/10.2307/2218153) and [Cook and Zhang (2015)](https://doi.org/10.1093/biomet/asv025), came from an experiment that compared two treatments for the control of a parasite in cattle. The experimenters were interested in finding if the treatments had differential effects on weight and, if so, about when they first occurred. There were sixty animals in this experiment and thirty animals were randomly assigned to the two treatments. Their weights (in kilograms) were then recorded at weeks 2, 4,..., 18 and 19 after treatment ([Kenward, 1987](https://doi.org/10.2307/2218153)). In our analysis, we considered the multivariate linear model (1), where $Y_i \in \mathbb{R}^{10}$ is the vector of cattle weights from week 2 to week 19, and predictor $X_i$ is either 0 or 1 indicating which of the two treatments was assigned. In this model, $\alpha$ is the mean profile for one treatment and $\beta$ is the mean difference between the two treatments.

Since the two treatments were not expected to have an immediate measurable affect on weight, some linear combinations of the response vector are not expected to depend on the treatment. Therefore the envelope model (3) is expected to perform well in this application because of our belief that (2) holds with $\hat{E}_2(B)$ at least as large as the span of the linear combinations that isolate the first few elements of the response vector.
Envelope models were fitted at each dimension from 1 to 10. The likelihood ratio test selected $\hat{u} = 1$ and BIC selected $\hat{u} = 3$ as the dimension of the envelope model. Further complicating matters, when BIC is used to determine $u$ at every resample of the multivariate residual bootstrap with sample size $B = 60$, we see high variability in the models selected. Specifically, $n(\hat{u} = 1) = 10$, $n(\hat{u} = 2) = 10$, $n(\hat{u} = 3) = 24$, $n(\hat{u} = 4) = 12$, and $n(\hat{u} = 5) = 4$. Model selection variability of this variety is precisely the reason why the weighted envelope estimator is advocated.

In Table 3, we see the ratios of bootstrapped estimated standard errors for envelope estimators to those of the maximum likelihood estimator of the $\beta$ from the full model $\beta$. Standard errors of the averaged ratios across replications are all less than 7% of the reported ratios and the average standard error is 2.6% of the reported ratio. Ratios greater than 1 indicate that the envelope estimator is more efficient than the standard estimator. We see that $\hat{\beta}_w$ is comparable to $\hat{\beta}_{u=3}$. Similar conclusions are drawn from the other elements of estimates of $\beta$. The findings displayed in Table 3 illustrate that the weighted envelope estimator can provide useful efficiency gains while properly accounting for model selection variability.

| $B$  | $\hat{\beta}_{u=1}$ | $\hat{\beta}_{u=2}$ | $\hat{\beta}_{u=3}$ | $\hat{\beta}_{u=4}$ | $\hat{\beta}_{u=5}$ |
|------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 60   | 1.98                | 5.54                | 3.05                | 1.69                | 1.31                |
| 100  | 1.97                | 5.54                | 2.55                | 1.54                | 1.32                |
| 500  | 1.82                | 5.47                | 2.78                | 1.57                | 1.31                |
| 2000 | 1.81                | 5.37                | 2.60                | 1.53                | 1.29                |

Table 3: Averaged ratios of estimated standard errors across 25 replications of the multivariate residual bootstrap at different numbers of resamples $B$ for the fifth element of estimates of $\beta$. Standard errors of the averaged ratios are in parentheses.

We next report results of a simulation study using the cattle data to show further support for Theorem 1. We generate data according to the model $Y_i = \alpha + \beta X_i + \varepsilon_i$, $\varepsilon_i \sim N(0, \Sigma)$, $(i = 1, \ldots, n)$ where $\alpha$, $\beta$, and $\Sigma$ were set to the estimates obtained from the envelope model fit to the cattle data at dimension $u = 3$, and $X_i$ is the binary indicator that specified treatment. Cows are split evenly between the two treatment groups and the assignment was random.

In Table 3 we see that the Euclidean differences between vec($\hat{\beta}_{u=3}$) and vec($\hat{\beta}_w$) shrink as $n$ increases. The same is true for the differences between vec($\hat{\beta}_{u=4}$) and vec($\hat{\beta}_w$). This was expected since the envelope model fit with $u = 4$ is a true data generating model. However, we see that the Euclidean distance between vec($\hat{\beta}_{u=2}$) and vec($\hat{\beta}_w$) does not shrink as $n$ increases. Again, this was expected since the envelope model fit with $u = 2$ is not a true data generating model. These simulation results are in alignment with the conclusions of Theorem 1.
\[ n = 60 \quad n = 100 \quad n = 500 \quad n = 2000 \]
\[
\begin{align*}
|\text{vec}(\hat{\beta}_w) - \text{vec}(\hat{\beta}_{u=2})|_2 & \quad 9.36 & 0.83 & 0.91 & 4.2 \\
|\text{vec}(\hat{\beta}_w) - \text{vec}(\hat{\beta}_{u=3})|_2 & \quad 9.37 & 0.54 & 0.070 & 0.00028 \\
|\text{vec}(\hat{\beta}_w) - \text{vec}(\hat{\beta}_{u=4})|_2 & \quad 9.37 & 0.69 & 0.34 & 0.090 
\end{align*}
\]

Table 4: Comparison of $\hat{\beta}_w$ and $\hat{\beta}_{u=2}$, $\hat{\beta}_{u=3}$, and $\hat{\beta}_{u=4}$. The rows are the Euclidean difference between vec($\hat{\beta}_w$) and the indicated envelope estimator from the original dataset.

## 6 Discussion

Efron (2014) proposed an estimator motivated by bagging (Breiman, 1996) that aims to reduce variability and smooth out discontinuities resulting from model selection volatility. Variability of the model averaged estimator of Efron (2014) is assessed via a double bootstrap. These techniques have been applied to envelope methodology in Eck, et al. (2016) and useful variance reduction was found empirically. The problem of interest in Eck, et al. (2016) falls outside the scope of the multivariate linear regression model, and general envelope methodology (Cook and Zhang, 2015) was required to obtain efficiency gains. In the context of the multivariate linear regression model, we showed that only a single level of bootstrapping is necessary.

The idea of weighting envelope estimators across all candidate dimensions extends to partial least squares (Cook, et al., 2013), predictor envelopes (Cook and Su, 2016), and sparse response envelopes (Su, et al., 2016).

## 7 Supplementary material

Supplementary material available at Biometrika online includes the proof of Theorem 1 and a complete version of Table 3 that includes standard errors for all of the averaged ratios.

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‘Supplementary material for Weighted envelope estimation to handle variability in model selection’

This Supplementary Materials section contains the proof of Theorem 1 and an extended version of Table 3 in Eck and Cook (2017).

In Table 5 we see the ratios of bootstrapped estimated standard errors between envelope estimators to those of the maximum likelihood estimator of the \( \beta \) from the full model (1), se* \( (\hat{\beta}_j)/\text{se}(\hat{\beta}_w) \), averaged across 25 replications. Standard errors of the averaged ratios across replications are in parentheses.

| \( B \) | \( \hat{\beta}_w \) | \( \hat{\beta}_{u=1} \) | \( \hat{\beta}_{u=2} \) | \( \hat{\beta}_{u=3} \) | \( \hat{\beta}_{u=4} \) | \( \hat{\beta}_{u=5} \) |
|------|------|------|------|------|------|------|
| 60   | 1.98 (0.081) | 5.54 (0.14) | 3.05 (0.19) | 1.69 (0.11) | 1.31 (0.044) | 1.23 (0.039) |
| 100  | 1.97 (0.10) | 5.54 (0.14) | 2.55 (0.15) | 1.54 (0.044) | 1.32 (0.038) | 1.21 (0.027) |
| 500  | 1.82 (0.031) | 5.47 (0.074) | 2.78 (0.076) | 1.57 (0.024) | 1.31 (0.013) | 1.16 (0.013) |
| 2000 | 1.81 (0.017) | 5.37 (0.049) | 2.60 (0.032) | 1.53 (0.013) | 1.29 (0.0084) | 1.16 (0.0071) |

Table 5: Averaged ratios of estimated standard errors across 25 replications of the multivariate residual bootstrap at different numbers of resamples \( B \) for the fifth element of estimates of \( \beta \). Standard errors of the averaged ratios are in parentheses.

Here is the proof of Theorem 1 in Eck and Cook (2017):

**Proof.** We go through the steps showing that (7) in Eck and Cook (2017) holds. Recall that \( u = \text{dim}(\mathcal{E}) \). Define \( l(\hat{\beta}_j) \) to be the log likelihood of the envelope model evaluated at the envelope estimator \( \hat{\beta}_j \), fitting with \( \text{dim}(\mathcal{E}) = j \), and define \( k(j) \) to be the number of parameters of the envelope model of dimension \( j \). From the construction of \( b_j \) and the above calculations we see that

\[
e^{b_u - b_j} = e^{-2\{l(\hat{\beta}_u) - l(\hat{\beta}_j)\} + n^{-2(k(j) - k(u))}}.
\]

Let \( b^*_j \) be the BIC value of the envelope model of dimension \( j \) fit to the starred data and define

\[
w^*_j = \frac{e^{-b^*_j}}{\sum_{k=1}^{r} e^{-b^*_k}}.
\]

Let \( \| \cdot \| \) be the Euclidean norm. We show that \( \sqrt{n} \{ w^*_j \vec{\beta}_j - w_j \vec{\beta}_j \} \rightarrow 0 \) for \( j \neq u \) by showing that

\[
\sqrt{n} \| w^*_j \vec{\beta}_j - w_j \vec{\beta}_j \| \leq \sqrt{n} \| w^*_j \vec{\beta}_j \| + \sqrt{n} \| w_j \vec{\beta}_j \| \rightarrow 0
\]

as \( n \rightarrow \infty \) for all \( j \neq u \). Now,

\[
\sqrt{n} w_j \| \vec{\beta}_j \| \leq \sqrt{n} \| O_p(1) \| e^{b_u - b_j} = |O_p(1)| \| n^{(k(u) - k(j) + 1/2)} e^{-2\{l(\hat{\beta}_u) - l(\hat{\beta}_j)\}}
\]

\[
= |O_p(1)| n^{(k(u) - k(j) + 1/2)} e^{2\{l(\hat{\beta}_u) - l(\hat{\beta}_u)\} - 2\{l(\hat{\beta}_u) - l(\hat{\beta}_j)\}}.
\]

(12)
The first inequality in (12) follows from the fact that \( \| \text{vec}(\hat{\beta}_j) \| \leq \| \text{vec}(\hat{\beta}_r) \| \) and \( \| \text{vec}(\hat{\beta}_r) \| = O_p(1) \). We first consider the case where \( j = u + 1, ..., r \). In this setting, models with envelope dimensions \( u \) and \( j \) are both true and nested within the full model with envelope dimension \( r \). Consequently, \( -2\{l(\hat{\beta}_u) - l(\hat{\beta}_r)\} \) and \( -2\{l(\hat{\beta}_j) - l(\hat{\beta}_r)\} \) are asymptotically distributed as \( \chi^2_{n_p(r-u)} \) and \( \chi^2_{p(r-j)} \) by Wilks’ Theorem. Therefore \( e^{-2\{l(\hat{\beta}_u) - l(\hat{\beta}_r)\}} = O_p(1) \) since it is the exponentiation of the difference between two \( \chi^2 \) random variables. We see that

\[
\sqrt{n w_j} \| \text{vec}(\hat{\beta}_j) \| \leq O_p(1) | n^{(k(u) - k(j) + 1/2)} = O_p \left[ n^{(k(u) - k(j) + 1/2)} \right].
\]

Since \( j > u \), we have that \( k(u) - k(j) = p(u - j) \leq -p \). Thus,

\[
\sqrt{n w_j} \| \text{vec}(\hat{\beta}_j) \| \leq O_p \left\{ n^{(1/2 - p)} \right\}
\]

for \( j = u + 1, ..., r \). Following the same steps as (12), applied to the starred data, yields

\[
\sqrt{n w_j^*} \| \text{vec}(\hat{\beta}_j^*) \| \leq O_p(1) | n^{(k(u) - k(j) + 1/2)} \left\{ n^{(k(u) - k(j) + 1/2)} \right\}
\]

\[= -2\left\{ l^*(\hat{\beta}_u^*) - l^*(\hat{\beta}_r^*) \right\} + 2\left\{ l^*(\hat{\beta}_j^*) - l^*(\hat{\beta}_r^*) \right\} \] in (13) are \( O_p(1) \). Thus,

\[
\sqrt{n w_j} \| \text{vec}(\hat{\beta}_j^*) \| \leq O_p \left\{ n^{(1/2 - p)} \right\} \text{ for all } j = u + 1, ..., r \].

This establishes that

\[
n \sqrt{n w_j^*} \text{vec}(\hat{\beta}_j^*) - w_j \text{vec}(\hat{\beta}_j) \| \leq O_p \left\{ n^{(1/2 - p)} \right\},
\]

for \( j = u + 1, ..., r \).

Turning to the case when \( j = 1, ..., u - 1, \) consider the exponent \( e^{-\lambda_j} \), with \( \lambda_j = -2 \{ l(\hat{\beta}_u) - l(\hat{\beta}_j) \} \). This is a log likelihood ratio although, unlike the case when \( j = u + 1, ..., r \), it does not follow a \( \chi^2 \) distribution asymptotically. Let \( \hat{G}_r \) and \( \hat{G}_o_r \) be the estimated bases for the envelope space and its orthogonal complement fitting with dimension \( j = 1, ..., u - 1, \) so \( \hat{G}_r \in \mathbb{R}^{r \times j} \) and \( \hat{G}_o_r \in \mathbb{R}^{r \times (r-j)} \). We write

\[
\lambda_j = -2 \{ l(\hat{\beta}_u) - l(\hat{\beta}_j) \} = n \log | \hat{G}_r^T \hat{\Sigma}_{\hat{r}} \hat{G}_r | + n \log | \hat{G}_o_r^T \hat{\Sigma}_r \hat{G}_o_r | - n \log | \hat{\Sigma}_r | - n \log | \hat{\Sigma}_{\hat{r}} | - n \log | \hat{\Sigma}_{\hat{r}} | + n \log | I_p + \hat{\Sigma}_r \hat{\beta}_r^T \hat{G}_o_r (\hat{G}_o_r^T \hat{\Sigma}_{\hat{r}} \hat{G}_o_r)^{-1} \hat{G}_o_r \hat{\beta}_r \hat{\Sigma}_{\hat{r}}^{1/2} |.
\]

where \( \hat{\Sigma}_Y = n^{-1} Y^T Y \). The second equation in (14) follows by applying the usual expansion of the determinant of a sum of the form \( A + BB^T \). To see this,

\[
| \hat{G}_o_r^T \hat{\Sigma}_r \hat{G}_o_r | = | \hat{G}_o_r^T \hat{\Sigma}_{\hat{r}} \hat{G}_o_r + \hat{G}_o_r^T \hat{\Sigma}_Y \hat{X}(X^T \hat{X})^{-1} X^T \hat{Y} \hat{G}_o_r |
\]

\[
= | \hat{G}_o_r^T \hat{\Sigma}_{\hat{r}} \hat{G}_o_r + \hat{G}_o_r^T \hat{\beta}_r \hat{\Sigma}_X \hat{\beta}_r^T \hat{G}_o_r |
\]

\[
= | \hat{G}_o_r^T \hat{\Sigma}_{\hat{r}} \hat{G}_o_r | \times | I_p + \hat{\Sigma}_X^{1/2} \hat{\beta}_r^T \hat{G}_o_r (\hat{G}_o_r^T \hat{\Sigma}_{\hat{r}} \hat{G}_o_r)^{-1} \hat{G}_o_r \hat{\beta}_r \hat{\Sigma}_X^{1/2} |
\]

where \( \hat{G}_o_r \hat{\beta}_r \hat{\Sigma}_X \hat{\beta}_r^T \hat{G}_o_r = \hat{G}_o_r^T \hat{\Sigma}_Y \hat{X}(X^T \hat{X})^{-1} X^T \hat{Y} \hat{G}_o_r \) because of the definition of \( \hat{\beta}_r = \hat{\beta}_r \hat{\Sigma}_X \hat{\beta}_r^T \hat{G}_o_r \).
We bound \( \lambda_j \) from below by further minimizing the first three addends in (14) over \((\tilde{G}, \tilde{G}_o)\). These are minimized globally when the columns of \( \tilde{G} \) span any reducing subspace of \( \tilde{\Sigma}_{\text{res}} \) and is 0 at the minimum. Thus

\[
\lambda_j \geq n \log | I_p + \left[ \tilde{G}_o^T \tilde{G}_o \right]^{-1} \tilde{G}_o^T \tilde{\beta} \tilde{X}^1/2 | \\
= n \log | I_p + \left[ \tilde{G}_o^T \tilde{G}_o \right]^{-1} \tilde{G}_o^T \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{\Sigma}_{\text{res}}^{-1/2} | \\
= n \log (\tilde{A}_{j,n}),
\]

where \( \tilde{A}_{j,n} \) is defined implicitly. The quantity \( \tilde{G}_o^T \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o \) in (15) is the projection into the column space of \( \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o \). The quantity \( \tilde{G}_o^T \tilde{\beta}_r \neq 0 \) almost surely since \( j = 1, \ldots, u - 1 \). As a result, the column space of \( \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{\beta}_r \tilde{X}^1/2 \) in (15) has a nontrivial intersection with the column space of \( \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o \) almost surely. Therefore \( \tilde{A}_{j,n} > 1 \) almost surely. We can write \( n \log (\tilde{A}_{j,n}) = n | O_p(1) | \) and we have the bound

\[
e^{-\lambda_j} = e^{-2(l(\tilde{\beta}_r) - l(\tilde{\beta}_r))} \leq e^{-n \log (\tilde{A}_{j,n})} = e^{-n | O_p(1) |}.\]

Therefore,

\[
\log (w_j) \leq b_u - b_j \\
= -2 \{ l(\tilde{\beta}_u) - l(\tilde{\beta}_u) \} + 2 \{ l(\tilde{\beta}_j) - l(\tilde{\beta}_j) \} + \{ k(u) - k(j) \} \log (n) \\
= | O_p(1) | - \lambda_j + \{ k(u) - k(j) \} \log (n) \\
\leq | O_p(1) | - n | O_p(1) | + \{ k(u) - k(j) \} \log (n) = -n | O_p(1) |
\]

and we see that \( \sqrt{n} w_j \leq \sqrt{n e^{-n | O_p(1) |}} \) for \( j = 1, \ldots, u - 1 \).

Define \( \tilde{G}_o^* \) to be the estimate of \( G_o \) obtained from the starred data and let

\[
\tilde{A}_{j,n}^* = | I_p + \left[ \tilde{G}_o^* \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o^* \right]^{-1} \tilde{G}_o^* \tilde{\beta}_r \tilde{X}^1/2 | \\
= | I_p + \left[ \tilde{G}_o^* \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o^* \right]^{-1} \tilde{G}_o^* \tilde{\Sigma}_{\text{res}}^{-1/2} | \\
\]

(17)

The same logic that applied to \( \tilde{A}_{j,n} \) applies to \( \tilde{A}_{j,n}^* \). The quantity \( \tilde{G}_o^* \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o^* \) in (17) is the projection onto the column space of \( \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o^* \). The quantity \( \tilde{G}_o^* \tilde{\beta}_r \neq 0 \) almost surely since \( j = 1, \ldots, u - 1 \). As a result, the column space of \( \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{\beta}_r \tilde{X}^1/2 \) in (17) has a nontrivial intersection with the column space of \( \tilde{\Sigma}_{\text{res}}^{-1/2} \tilde{G}_o^* \) almost surely. Therefore \( \tilde{A}_{j,n}^* > 1 \) almost surely. The steps in (16), applied to the starred data, yields

\[
\sqrt{n} w_j^* \leq \sqrt{n e^{-n | O_p(1) |}}.
\]

Thus,

\[
\sqrt{n} w_j^* \vec{v}(\tilde{\beta}_j^*) - w_j \vec{v}(\tilde{\beta}_j) \leq \sqrt{n} w_j^* \vec{v}(\tilde{\beta}_j^*) + \sqrt{n} w_j \vec{v}(\tilde{\beta}_j) \\
\leq \sqrt{n e^{-n | O_p(1) |}} | \vec{v}(\tilde{\beta}_j^*) | + \sqrt{n e^{-n | O_p(1) |}} | \vec{v}(\tilde{\beta}_j) | \\
= 2 O_p(1) \sqrt{n e^{-n | O_p(1) |}}
\]

for \( j = 1, \ldots, u - 1 \) where \( | \vec{v}(\tilde{\beta}_j) | \) and \( | \vec{v}(\tilde{\beta}_j^*) | \) are both \( O_p(1) \) just as in the \( j = u + 1, \ldots, r \) case. Combining all of these terms yields the \( 2(u - 1) O_p(1) \sqrt{n e^{-n | O_p(1) |}} \) order in (7) in Eck and Cook (2017). This completes the proof when \( j = 1, \ldots, u - 1 \).
The final case is when \( j = u \). Let \( E_n = \sum_{i \neq u} e^{b_i - b_u} \). We can write \( w_u = \frac{1}{1 + E_n} = 1 - \frac{E_n}{1 + E_n} \). The term\( E_n = O_p(n^{-p}) \) since \( e^{-nO_p(1)} = O_p(n^{-p}) \). Therefore

\[
\sqrt{n} w_u^* \text{vec}(\hat{\beta}_u^*) = \sqrt{n} \left( 1 - \frac{E_n}{1 + E_n} \right) \text{vec}(\hat{\beta}_u^*)
\]

\[
= \sqrt{n} \text{vec}(\hat{\beta}_u^*) + O_p\left\{ n^{(1/2-p)} \right\},
\]

\[
\sqrt{n} w_u \text{vec}(\hat{\beta}_u) = \sqrt{n} \left( 1 - \frac{E_n}{1 + E_n} \right) \text{vec}(\hat{\beta}_u)
\]

\[
= \sqrt{n} \text{vec}(\hat{\beta}_u) + O_p\left\{ n^{(1/2-p)} \right\}.
\]

Adding the previous results over \( j \) to form \( \sqrt{n} \left\{ \text{vec}(\hat{\beta}_u^*) - \text{vec}(\hat{\beta}_u) \right\} \) yields the result given in (7) in Eck and Cook (2017). This completes the proof.

\[\square\]

References

Eck, D. J. and Cook, R. D. (2017). Weighted envelope estimation to handle variability in model selection. Submitted.