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Bootstrapping for multivariate linear regression models

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ABSTRACT

The multivariate linear regression model is an important tool for investigating relationships between several response variables and several predictor variables. The primary interest is in inference about the unknown regression coefficient matrix. We propose multivariate bootstrap techniques as a means for making inferences about the unknown regression coefficient matrix. These bootstrapping techniques are extensions of those developed in Freedman (1981), which are only appropriate for univariate responses. Extensions to the multivariate linear regression model are made without proof. We formalize this extension and prove its validity. A real data example and two simulated data examples which offer some finite sample verification of our theoretical results are provided.

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1. Introduction

The linear regression model is an important and useful tool in many statistical analyses for studying the relationship among variables. Regression analysis is primarily used for predicting values of the response variable at interesting values of the predictor variables, discovering the predictors that are associated with the response variable, and estimating how changes in the predictor variables affects the response variable (Weisberg, 2005). The standard linear regression methodology assumes that the response variable is a scalar. However, it may be the case that one is interested in investigating multiple response variables simultaneously. One could perform a regression analysis on each response separately in this setting. Such an analysis would fail to detect associations between responses. Regression settings where associations of multiple responses are of interest require a multivariate linear regression model for analysis.

Bootstrapping techniques are well understood for the linear regression model with a univariate response (Bickel and Freedman, 1981; Freedman, 1981). In particular, theoretical justification for the residual bootstrap as a way to estimate the variability of the ordinary least squares (OLS) estimator of the regression coefficient vector in this model has been developed (Freedman, 1981). Theoretical extensions of residual bootstrap techniques appropriate for the multivariate linear regression model have not been formally introduced. The existence of such an extension is stated without proof and rather implicitly in subsequent works (Freedman and Peters, 1984; Diaconis and Efron, 1983). In this article we show that the bootstrap procedures in Freedman (1981) provide consistent estimates of the variability of the OLS estimator of the regression coefficient matrix in the multivariate linear regression model. Our proof technique follows similar logic as Freedman (1981). The generality of the bootstrap theory developed in Bickel and Freedman (1981) provide the tools required for our extension to the multivariate linear regression model.

2. Bootstrap for the multivariate linear regression model

The multivariate linear regression is

$$Y_i = \beta X_i + \varepsilon_i, \quad (i = 1, \dots, n), \quad (1)$$

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where $Y_i \in \mathbb{R}^r$ and $r > 1$ in order to have an interesting problem, $\beta \in \mathbb{R}^{r \times p}$, $X_i \in \mathbb{R}^p$, and the ε_i 's $\in \mathbb{R}^r$ are errors having mean zero and variance–covariance matrix Σ where $\Sigma > 0$. It is assumed that separate realizations from the model (1) are independent and that $n > p$. We further define $\mathbb{X} \in \mathbb{R}^{n \times p}$ as the design matrix with rows X_i^T , $\mathbb{Y} \in \mathbb{R}^{n \times r}$ is the matrix of responses with rows Y_i^T , and $\varepsilon \in \mathbb{R}^{n \times r}$ is the matrix of all errors with rows ε_i^T . The OLS estimator of β in model (1) is $\hat{\beta} = \mathbb{Y}^T \mathbb{X} (\mathbb{X}^T \mathbb{X})^{-1}$. We let $\hat{\varepsilon} \in \mathbb{R}^{n \times r}$ denote the matrix of residuals consisting of rows $\hat{\varepsilon}_i^T = (Y_i - \hat{\beta} X_i)^T$. The multivariate linear regression model assumed here is slightly different than the traditional multivariate linear regression model. The traditional model makes the additional assumptions that the errors are normally distributed and the design matrix \mathbb{X} is fixed.

We consider two bootstrap procedures that consistently estimate the asymptotic variability of $\text{vec}(\hat{\beta})$ under different assumptions placed upon the model (1), where the vec operator stacks the columns of a matrix so that $\text{vec}(\beta) \in \mathbb{R}^{rp \times 1}$. The first bootstrap procedure is appropriate when the design matrix \mathbb{X} is assumed to be fixed and the errors are constant. In this setup, residuals are resampled. The second bootstrap procedure is appropriate when $(X_i^T, \varepsilon_i^T)^T$ are realizations from a joint distribution. In this setup, cases $(X_i^T, Y_i^T)^T$ are resampled. It is known that bootstrapping under these setups provides a consistent estimator of the variability of $\text{var}(\hat{\beta})$ in model (1) when $r = 1$ (Freedman, 1981). Convergence theorems are stated in terms of the Mallows metric for two probability measures μ, ν in \mathbb{R}^k . The Mallows metric is

$$d_1^p(\mu, \nu) = \inf_{U \sim \mu, V \sim \nu} E^{1/p} (\|U - V\|^p). \quad (2)$$

A brief description of useful properties of (2) is stated in the beginning of Section 4. We now provide the needed multivariate bootstrap extensions.

2.1. Fixed design

We first establish the residual bootstrap of Freedman (1981) when \mathbb{X} is assumed to be a fixed design matrix. Resampled, starred, data is generated by the model

$$\mathbb{Y}^* = \mathbb{X} \hat{\beta}^T + \varepsilon^*, \quad (3)$$

where $\varepsilon^* \in \mathbb{R}^{n \times r}$ is the matrix of errors with rows being independent. The rows in ε^* have common distribution \hat{F}_n which is the empirical distribution of the residuals from the original dataset, centered at their mean. Now $\hat{\beta}^* = \mathbb{Y}^{*T} \mathbb{X} (\mathbb{X}^T \mathbb{X})^{-1}$ is the OLS estimator of β from the starred data. This process is performed a total of B times with a new estimator $\hat{\beta}^*$ computed from (3) at each iteration. We then estimate the variability of $\text{vec}(\hat{\beta})$ with

$$\text{var}^* \left\{ \text{vec}(\hat{\beta}) \right\} = (B-1)^{-1} \sum_{b=1}^B \left\{ \text{vec}(\hat{\beta}_b^*) - \text{vec}(\bar{\beta}^*) \right\} \left\{ \text{vec}(\hat{\beta}_b^*) - \text{vec}(\bar{\beta}^*) \right\}^T$$

where $\hat{\beta}_b^*$ is the residual bootstrap estimator of β at iteration b and $\bar{\beta}^* = B^{-1} \sum_{b=1}^B \hat{\beta}_b^*$. We summarize this bootstrap procedure in Algorithm 1.

Algorithm 1. Bootstrap procedure with fixed design matrix.

- Step 1. Set B and initialize $b = 1$.
- Step 2. Sample residuals from \hat{F}_n , with replacement, and compute \mathbb{Y}^* as in (3).
- Step 3. Compute $\hat{\beta}_b^* = \mathbb{Y}^{*T} \mathbb{X} (\mathbb{X}^T \mathbb{X})^{-1}$, store $\text{vec}(\hat{\beta}_b^*)$, and let $b = b + 1$.
- Step 4. Repeat Steps 2–3 $B - 1$ times.

Before the theoretical justification of the residual bootstrap is formally given, some important quantities are stated. The residuals from the regression (3) are $\hat{\varepsilon}^* = \mathbb{Y}^* - \mathbb{X} \hat{\beta}^{*T}$. The variance–covariance matrix Σ in model (1) is then estimated by

$$\hat{\Sigma} = n^{-1} \sum_{i=1}^n \hat{\varepsilon}_i \hat{\varepsilon}_i^T - \hat{\mu}^2, \quad \hat{\mu}^2 = \left(n^{-1} \sum_{i=1}^n \hat{\varepsilon}_i \right) \left(n^{-1} \sum_{i=1}^n \hat{\varepsilon}_i \right)^T.$$

Likewise, the variance–covariance estimate from the starred data is

$$\hat{\Sigma}^* = n^{-1} \sum_{i=1}^n \hat{\varepsilon}_i^* \hat{\varepsilon}_i^{*T} - \hat{\mu}^{*2}, \quad \hat{\mu}^{*2} = \left(n^{-1} \sum_{i=1}^n \hat{\varepsilon}_i^* \right) \left(n^{-1} \sum_{i=1}^n \hat{\varepsilon}_i^* \right)^T.$$

Let I_k denote the $k \times k$ identity matrix. Theorem 1 provides bootstrap asymptotics for the regression model (1). It extends Theorem 2.2 of Freedman (1981) to the multivariate setting.

Theorem 1. Assume the regression model (1) where the errors have finite fourth moments. Suppose that $n^{-1} \mathbb{X}^T \mathbb{X} \rightarrow \Sigma_X > 0$. Then, conditional on almost all sample paths Y_1, \dots, Y_n , as $n \rightarrow \infty$,

- (a) $d_2^p \left[\sqrt{n} \left\{ \text{vec}(\hat{\beta}^*) - \text{vec}(\hat{\beta}) \right\}, N(0, \Sigma_X^{-1} \otimes \Sigma) \right] \rightarrow 0$,
 (b) $\hat{\Sigma}^* \rightarrow_p \Sigma$, and
 (c) $d_2^p \left[\sqrt{n} \left\{ (\mathbb{X}^T \mathbb{X})^{1/2} \otimes \hat{\Sigma}^{*-1/2} \right\} \left\{ \text{vec}(\hat{\beta}^*) - \text{vec}(\hat{\beta}) \right\}, N(0, I_{rp}) \right] \rightarrow 0$.

The proof of [Theorem 1](#), along with the details of several necessary lemmas and theorems, are included in the theoretical details section. [Theorem 1](#) establishes the multivariate analogue for the residual bootstrap. This theorem shows that standard error estimation of the estimated β matrix obtained through bootstrapping, is \sqrt{n} -consistent. Now let $f : \mathbb{R}^p \rightarrow \mathbb{R}^k$ be a differentiable function. Then the conclusions of [Theorem 1](#) can be applied to establish a multivariate delta method based on estimates obtained via the residual bootstrap. This immediately follows from a first order Taylor expansion and some algebra arriving at

$$\sqrt{n} \left[f \left\{ \text{vec}(\hat{\beta}^*) \right\} - f \left\{ \text{vec}(\hat{\beta}) \right\} \right] = \nabla f \left\{ \text{vec}(\hat{\beta}) \right\} \sqrt{n} \left\{ \text{vec}(\hat{\beta}^*) - \text{vec}(\hat{\beta}) \right\} + O_p(n^{-1/2}). \quad (4)$$

Therefore (4) converges weakly to a normal distribution with mean zero and variance given by

$$\nabla f \left\{ \text{vec}(\beta) \right\} (\Sigma_X^{-1} \otimes \Sigma) \nabla^T f \left\{ \text{vec}(\beta) \right\}$$

as $n \rightarrow \infty$.

2.2. Random design and heteroskedasticity

In this section we assume that the X_i s in model (1) are realizations of a random variable X . The regression coefficient matrix β now takes the form $\beta = E(YX^T)\Sigma_X^{-1}$ where $\Sigma_X = E(XX^T)$ and it is assumed that $\Sigma_X > 0$. Now that X is stochastic, there may be some association between X and the errors ε . The possibility of heteroskedasticity means that we need to alter the bootstrap procedure outlined in the previous section in order to consistently estimate the variability of $\text{vec}(\hat{\beta})$.

It is assumed that the data vectors $(X_i^T, Y_i^T)^T \in \mathbb{R}^{p+r}$ are independent, with a common distribution μ and $E(\|(X_i^T, Y_i^T)^T\|^4) < \infty$ where $\|\cdot\|$ is the Euclidean norm. Unlike the fixed design setting, data pairs $(X_i^T, Y_i^T)^T$ are resampled with replacement to form the starred data $(X_i^{*T}, Y_i^{*T})^T$, for $i = 1, \dots, n$. Given the original sample, $(X_i^T, Y_i^T)^T$, $i = 1, \dots, n$, the resampled vectors are independent, with distribution μ_n . Denote $\mathbb{X}^* \in \mathbb{R}^{n \times p}$ and $\mathbb{Y}^* \in \mathbb{R}^{n \times r}$ as the matrix with rows X_i^{*T} and Y_i^{*T} respectively. The starred estimator of β obtained from resampling is then $\hat{\beta}^* = \mathbb{Y}^{*T} \mathbb{X}^* (\mathbb{X}^{*T} \mathbb{X}^*)^{-1}$. For every n there is positive probability, albeit low, that $\mathbb{X}^{*T} \mathbb{X}^*$ is singular, and the probability of singularity decreases exponentially in n . We assume that displayed equation (1.17) in [Chatterjee and Bose \(2000\)](#) holds in order to circumvent singularity in our bootstrap procedure.

The bootstrap is performed a total of B times with a new estimator $\hat{\beta}^*$ computed at each iteration. We then estimate the variability of $\text{vec}(\hat{\beta})$ with

$$\text{var}^* \left\{ \text{vec}(\hat{\beta}) \right\} = (B-1)^{-1} \sum_{b=1}^B \left\{ \text{vec}(\hat{\beta}_b^*) - \text{vec}(\bar{\beta}^*) \right\} \left\{ \text{vec}(\hat{\beta}_b^*) - \text{vec}(\bar{\beta}^*) \right\}^T$$

where $\hat{\beta}_b^*$ is the bootstrap estimator of β at iteration b and $\bar{\beta}^* = B^{-1} \sum_{b=1}^B \hat{\beta}_b^*$. We summarize this bootstrap procedure in [Algorithm 2](#).

Algorithm 2. Bootstrap procedure with random design matrix.

- Step 1. Set B and initialize $b = 1$.
- Step 2. Resample $(X_i^T, Y_i^T)^T$ with replacement.
- Step 3. Compute $\hat{\beta}_b^* = \mathbb{Y}^{*T} \mathbb{X}^* (\mathbb{X}^{*T} \mathbb{X}^*)^{-1}$, store $\text{vec}(\hat{\beta}_b^*)$ and let $b = b + 1$.
- Step 4. Repeat Steps 2–3 $B - 1$ times.

We now show that the variability of $\text{vec}(\hat{\beta})$ is estimated consistently by our multivariate bootstrap procedure which resamples cases. Let M be a non-negative definite matrix with entries $M_{jk} = E \left\{ \text{vec}(X_i \varepsilon_i^T)_j \text{vec}(X_i \varepsilon_i^T)_k \right\}$ for $j, k = 1, \dots, rp$ and define $\Delta = (\Sigma_X^{-1} \otimes I_r) M (\Sigma_X^{-1} \otimes I_r)$. where $n^{-1} \mathbb{X}^T \mathbb{X} \rightarrow \Sigma_X$ a.e. as $n \rightarrow \infty$. Then

$$\begin{aligned} \sqrt{n} \text{vec}(\hat{\beta} - \beta) &= \text{vec} \left\{ n^{-1/2} \varepsilon^T \mathbb{X} (n^{-1} \mathbb{X}^T \mathbb{X})^{-1} \right\} \\ &= \left\{ (n^{-1} \mathbb{X}^T \mathbb{X})^{-1} \otimes I_r \right\} \text{vec} \left(n^{-1/2} \varepsilon^T \mathbb{X} \right) \rightarrow N(0, \Delta). \end{aligned} \quad (5)$$

The next theorem states that $\sqrt{n} \text{vec}(\hat{\beta}^* - \hat{\beta})$ is the same as (5). This is an extension of [Theorems 3.1 and 3.2 of Freedman \(1981\)](#) to the multivariate linear regression setting.

Theorem 2. Assume that $(X_i^T, Y_i^T)^T \in \mathbb{R}^{p+r}$ are independent, with a common distribution μ , $E(\|(X_i^T, Y_i^T)^T\|^4) < \infty$, and $\Sigma_X = E(XX^T)$ is positive definite. Then, conditional on almost all sample paths, $(X_i^T, Y_i^T)^T$, $i = 1, \dots, n$, as $n \rightarrow \infty$,

Table 1

Comparison of the 95% confidence interval obtained by the bootstrap using [Algorithm 1](#) (column 2) and a 95% confidence interval obtained by maximum likelihood estimation (column 3) for the first two components of $\text{vec}(\beta)$ (column 1).

	Component	Bootstrap CI	Sample CI
$n = 100$	$\text{vec}(\beta)_1$	(−0.517 0.831)	(−0.502 0.843)
	$\text{vec}(\beta)_2$	(0.063 1.449)	(0.031 1.443)
$n = 500$	$\text{vec}(\beta)_1$	(0.406 0.950)	(0.401 0.955)
	$\text{vec}(\beta)_2$	(−0.172 0.342)	(−0.175 0.336)
$n = 1000$	$\text{vec}(\beta)_1$	(0.289 0.682)	(0.293 0.681)
	$\text{vec}(\beta)_2$	(0.102 0.487)	(0.100 0.490)
$n = 5000$	$\text{vec}(\beta)_1$	(0.481 0.656)	(0.480 0.656)
	$\text{vec}(\beta)_2$	(0.046 0.223)	(0.047 0.221)

$$(a) n^{-1} \left(\mathbb{X}^{*T} \mathbb{X}^* \right) \rightarrow_{p^*} \Sigma_X,$$

$$(b) d_2^{TP} \left[\sqrt{n} \left\{ \text{vec}(\hat{\beta}^*) - \text{vec}(\hat{\beta}) \right\}, N(0, \Delta) \right] \rightarrow 0, \text{ and}$$

$$(c) \text{ the sequence } \hat{\Sigma}^* \rightarrow_{p^*} \Sigma.$$

The proof of [Theorem 2](#), along with necessary lemmas, are included in the theoretical details section.

3. Examples

3.1. Simulations

In this section we provide two simulated examples which show support for our multivariate bootstrap procedures.

3.1.1. Fixed design

This example illustrates [Theorem 1](#). We generated data according to the multivariate linear regression model (1) where $Y_i \in \mathbb{R}^3, X_i \in \mathbb{R}^2$, and both β and Σ are prespecified. Our goal is to make inference about $\text{vec}(\beta)$ using confidence intervals. For each component of β , a 95% confidence interval computed using the residual bootstrap in [Algorithm 1](#) is compared with a 95% confidence interval obtained from maximum likelihood estimation of β and Σ in model (1). Four data sets were generated at different sample sizes and the performance of the multivariate residual bootstrap is assessed. The bootstrap is performed $B = 5000$ times in each dataset. The results are displayed in [Table 1](#). For the first two components of β , we see that the confidence regions obtained from both methods are close to each other and that the distance between the two shrinks as n increases. Similar results are obtained for the other components of β . A separate simulation study shows that the coverage probabilities of our bootstrap are at the nominal level for all of the considered cases.

3.1.2. Random design and heteroskedasticity

This example aims to show support for [Theorem 2](#). We generated data according to the multivariate linear regression model (1) where $Y_i \in \mathbb{R}^3, X_i \in \mathbb{R}^2$, and both β and Σ are prespecified. The predictors and errors are generated according to

$$\begin{pmatrix} X_i \\ \varepsilon_i \end{pmatrix} \sim N \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \Sigma_X & \Sigma_{X\varepsilon} \\ \Sigma_{\varepsilon X} & \Sigma \end{pmatrix} \right\},$$

for $i = 1, \dots, n$. Our goal is to make inference about $\text{vec}(\beta)$ using the multivariate bootstrap procedure in the random design case. For each component of β , a 95% confidence interval computed using the bootstrap in [Algorithm 2](#) is compared with a 95% confidence interval obtained from maximum likelihood estimation of β and Σ in model (1) under heterogeneity. Four data sets were generated at different sample sizes and the performance of the multivariate bootstrap is assessed. The bootstrap is performed a total of $B = 5000$ times in each dataset. The results are displayed in [Table 2](#). For the first two components of β , we see that the confidence regions obtained from both methods are close to each other and that the distance between the two shrinks as n increases. Similar results are obtained for the other components of β . A separate simulation study shows that the coverage probabilities of our bootstrap are at the nominal level for all of the considered cases.

3.2. Cars data

The data in this example, analyzed in [Henderson and Velleman \(1981\)](#), was extracted from the 1974 Motor Trend US magazine. The objective of this study is to compare aspects of automobile design on performance and fuel composition for 32 automobiles (1973–74) models. In this analysis, we assume that the multivariate model (1) with miles per gallon, displacement, and horse power as response variables and number of cylinders and transmission type are predictors. Number

Table 2

Comparison of the 95% confidence interval obtained by the bootstrap using [Algorithm 2](#) (column 2) and a 95% confidence interval obtained by maximum likelihood estimation (column 3) for the first two components of $\text{vec}(\beta)$ (column 1).

	Component	Bootstrap CI	Sample CI
$n = 100$	$\text{vec}(\beta)_1$	(0.098 1.282)	(0.145 1.230)
	$\text{vec}(\beta)_2$	(0.111 1.025)	(0.114 1.042)
$n = 500$	$\text{vec}(\beta)_1$	(0.987 1.505)	(0.995 1.505)
	$\text{vec}(\beta)_2$	(0.583 1.109)	(0.604 1.084)
$n = 1000$	$\text{vec}(\beta)_1$	(0.801 1.185)	(0.804 1.180)
	$\text{vec}(\beta)_2$	(0.620 0.983)	(0.635 0.968)
$n = 5000$	$\text{vec}(\beta)_1$	(0.945 1.117)	(0.944 1.118)
	$\text{vec}(\beta)_2$	(0.637 0.808)	(0.645 0.798)

Table 3

Comparison of the 95% confidence interval obtained by the bootstrap using [Algorithm 1](#) (column 2) and a 95% confidence interval obtained by maximum likelihood estimation (column 3) for the first five components of $\text{vec}(\beta)$ (column 1).

Component	Bootstrap CI	Sample CI
$\text{vec}(\beta)_1$	(2.271 7.108)	(2.286 7.136)
$\text{vec}(\beta)_2$	(−3.775 0.838)	(−3.806 0.916)
$\text{vec}(\beta)_3$	(−6.896 −3.846)	(−6.900 −3.812)
$\text{vec}(\beta)_4$	(0.176 4.967)	(0.181 4.939)
$\text{vec}(\beta)_5$	(−134.226 −55.706)	(−134.408 −56.787)

of cylinders and transmission type are both factor variables. The automobiles have either 4, 6, or 8 cylinders and their transmission type is either automatic or manual.

For inference for β , we compare a 95% bootstrap confidence interval using the fixed design bootstrap in [Algorithm 1](#) with a 95% confidence interval obtained from maximum likelihood estimation of β and Σ in model (1). The number of bootstrap resamples is set at $B = 5000$. The results are depicted in [Table 3](#). We see that inferences about β are fairly similar for both methods. This suggests that the multivariate linear model with constant errors and a fixed design is an appropriate model for the cars data.

4. Theoretical details

Before we present our proof of [Theorems 1](#) and [2](#), we motivate the Mallows metric as a central tool for our proof technique. The Mallows metric for probabilities in \mathbb{R}^p , relative to the Euclidean norm was the driving force needed to establish the validity of the residual bootstrap approximation in the context of univariate regression ([Bickel and Freedman, 1981](#); [Freedman, 1981](#)). Properties of the Mallows metric are developed for random variables on separable Banach spaces of finite dimension ([Bickel and Freedman, 1981](#)). Since \mathbb{R}^k is indeed a separable Banach space for a natural number k , the theory in [Bickel and Freedman \(1981\)](#) applies to our case. In the present article, we use the Mallows metric when $r > 1$ to prove that the residual bootstrap can be used to estimate the variability of $\text{vec}(\hat{\beta})$ consistently.

4.1. Fixed design

Let $\Psi_n(F)$ be the distribution function of $\sqrt{n} \{ \text{vec}(\hat{\beta}) - \text{vec}(\beta) \}$ where F is the law of the errors ε so that $\Psi_n(F)$ is a probability measure on \mathbb{R}^{np} . Let G be an alternate law of the errors, where it is assumed that G is mean-zero with finite variance $\Sigma_G > 0$. In applications, G will be the centered empirical distribution of the residuals.

Theorem 3. $[d_2^{rp} \{ \Psi_n(F), \Psi_n(G) \}]^2 \leq nr \text{tr} \{ (\mathbb{X}^T \mathbb{X})^{-1} \} \{ d_2^r(F, G) \}^2$.

Proof. Let $A = \mathbb{X}(\mathbb{X}^T \mathbb{X})^{-1}$. Then $\Psi_n(F)$ is the law of $\sqrt{n} \varepsilon_n^T(F)A$ where $\varepsilon_n(F)$ is the matrix with n rows of independent random variables ε , having common law F . $\Psi_n(G)$ can be thought of similarly. Observe that $A^T A = (\mathbb{X}^T \mathbb{X})^{-1}$. Then, from [Lemma 8.9](#) in [Bickel and Freedman \(1981\)](#), we see that

$$\begin{aligned} [d_2^{rp} \{ \Psi_n(F), \Psi_n(G) \}]^2 &= (d_2^{rp} [\text{vec}\{\varepsilon_n^T(F)A\}, \text{vec}\{\varepsilon_n^T(G)A\}])^2 \\ &= (d_2^{rp} [(A^T \otimes I_r) \text{vec}\{\varepsilon_n^T(F)\}, (A^T \otimes I_r) \text{vec}\{\varepsilon_n^T(G)\}])^2 \\ &\leq n \text{tr} \{ (A^T \otimes I_r)(A^T \otimes I_r)^T \} \{ d_2^r(F, G) \}^2 = n \text{tr} \{ (A^T \otimes I_r)(A \otimes I_r) \} \{ d_2^r(F, G) \}^2 \end{aligned}$$

$$\begin{aligned} &= n \operatorname{tr} (A^T A \otimes I_r) \{d_2^r(F, G)\}^2 = n \operatorname{tr} \{(\mathbb{X}^T \mathbb{X})^{-1} \otimes I_r\} \{d_2^r(F, G)\}^2 \\ &= nr \operatorname{tr} \{(\mathbb{X}^T \mathbb{X})^{-1}\} \{d_2^r(F, G)\}^2, \end{aligned}$$

which is our desired conclusion. \square

With [Theorem 3](#) we can bound the distance between the sample dependent distribution functions $\Psi_n(F)$ and $\Psi_n(G)$ by the distance between their underlying laws. As in [Freedman \(1981\)](#), we proceed with F_n as the empirical distribution function of $\varepsilon_1, \dots, \varepsilon_n$. Let \tilde{F}_n be the empirical distribution of the residuals $\hat{\varepsilon}_1, \dots, \hat{\varepsilon}_n$ from the original regression, and let \hat{F}_n be \tilde{F}_n centered at its mean $\hat{\mu} = n^{-1} \sum_{i=1}^n \hat{\varepsilon}_i$. Since $\hat{\varepsilon} = \mathbb{Y} - \mathbb{X}\hat{\beta}^T$, we have $\hat{\varepsilon} - \varepsilon = -\mathcal{P}\varepsilon$ where \mathcal{P} is the projection into the column space of \mathbb{X} .

Lemma 1. $E^2 \{d_2^r(\tilde{F}_n, F_n)\} \leq p \operatorname{tr}(\Sigma)/n$.

Proof. From the definition of the Mallows metric we have

$$\begin{aligned} \{d_2^r(\tilde{F}_n, F_n)\}^2 &\leq n^{-1} \sum_{i=1}^n \|\hat{\varepsilon}_i - \varepsilon_i\|^2 = n^{-1} \operatorname{tr} \{(\hat{\varepsilon} - \varepsilon)^T (\hat{\varepsilon} - \varepsilon)\} \\ &= n^{-1} \operatorname{tr} (\varepsilon^T \mathcal{P} \varepsilon). \end{aligned}$$

From linearity of the expectation with respect to the trace operator,

$$E \{ \operatorname{tr} (\varepsilon^T \mathcal{P} \varepsilon) \} = \operatorname{tr} \{ E (\varepsilon^T \mathcal{P} \varepsilon) \} = \operatorname{tr} \{ \mathcal{P} E (\varepsilon \varepsilon^T) \} \leq \operatorname{tr} (\mathcal{P}) \operatorname{tr} (\Sigma) = p \operatorname{tr} (\Sigma)$$

and this completes the proof. \square

Lemma 2. $E^2 \{d_2^r(\hat{F}_n, F_n)\} \leq (p+1) \operatorname{tr}(\Sigma)/n$.

Proof. From [Lemma 8.8](#) in [Bickel and Freedman \(1981\)](#) we have

$$\begin{aligned} d_2^r(\hat{F}_n, F_n)^2 &= d_2^r(\tilde{F}_n - E(\tilde{F}_n), F_n - E(F_n))^2 + \|E(F_n)\|^2 \\ &= d_2^r(\tilde{F}_n, F_n)^2 - \|E(\tilde{F}_n) - E(F_n)\|^2 + \|E(F_n)\|^2 \\ &\leq d_2^r(\tilde{F}_n, F_n)^2 + \|n^{-1} \sum_{i=1}^n \varepsilon_i\|^2 \end{aligned}$$

with the empirical distribution functions F_n , \tilde{F}_n , and \hat{F}_n used as random variables in the application of [Lemma 8.8](#) in [Bickel and Freedman \(1981\)](#). We see that

$$E \left(\left\| n^{-1} \sum_{i=1}^n \varepsilon_i \right\|^2 \right) = n^{-2} \left\{ E \left(\sum_{i=1}^n \varepsilon_i^T \varepsilon_i + \sum_{i \neq j} \varepsilon_i^T \varepsilon_j \right) \right\} = n^{-1} \{E(\varepsilon_1^T \varepsilon_1)\} = n^{-1} \operatorname{tr} (\Sigma).$$

Our conclusion follows from [Lemma 1](#). \square

These results imply the validity of the bootstrap approximation for the model [\(1\)](#) if we assume that $n^{-1} \mathbb{X}^T \mathbb{X} \rightarrow \Sigma_X > 0$. From [Theorem 3](#),

$$E [d_2^p \{\Psi_n(\hat{F}_n), \Psi_n(F)\}] \leq nr \operatorname{tr} \{(\mathbb{X}^T \mathbb{X})^{-1}\} d_2^r(\hat{F}_n, F)$$

and because of the metric properties of $d_2^r(\cdot, \cdot)$

$$\frac{1}{2} d_2^r(\hat{F}_n, F)^2 \leq d_2^r(\hat{F}_n, F_n)^2 + d_2^r(F_n, F)^2$$

where [Lemma 2](#) shows that $d_2^r(\hat{F}_n, F_n)^2 \rightarrow_p 0$ and [Lemma 8.4](#) of [Bickel and Freedman \(1981\)](#) implies that $d_2^r(F_n, F)^2 \rightarrow_p 0$ with the separable Banach space taken to be \mathbb{R}^r . The next results are special cases of [Lai et al. \(1979\)](#) which are adapted from [Freedman \(1981\)](#) to the multivariate setting. We let $\varepsilon_j, j = 1, \dots, r$, be the column of ε corresponding to the errors of response Y_j .

Lemma 3. $n^{-1} \mathbb{X}^T \varepsilon \rightarrow 0$ a.s. and $\hat{\beta} \rightarrow \beta$ a.s.

Proof. Let A_j be the j th column of ε . Then $n^{-1} \mathbb{X}^T \varepsilon \in \mathbb{R}^{p \times r}$ with columns $n^{-1} \mathbb{X}^T A_j$. [Lemma 2.3](#) of [Freedman \(1981\)](#) states that $n^{-1} \mathbb{X}^T A_j \rightarrow 0$ a.s. for any particular $j = 1, \dots, r$. Therefore $n^{-1} \mathbb{X}^T \varepsilon \rightarrow 0$ a.s. A similar argument verifies our second result. \square

Lemma 4. $n^{-1} \operatorname{tr} \{(\hat{\varepsilon} - \varepsilon)^T (\hat{\varepsilon} - \varepsilon)\} \rightarrow 0$ a.s.

Proof. A similar argument to that of Lemma 2.4 in Freedman (1981) gives

$$\begin{aligned} n^{-1} \operatorname{tr} \{(\widehat{\varepsilon} - \varepsilon)^T(\widehat{\varepsilon} - \varepsilon)\} &= n^{-1} \operatorname{tr} \{\varepsilon^T \mathbb{X}(\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \varepsilon\} \\ &= \operatorname{tr} \left\{ (n^{-1} \varepsilon^T \mathbb{X}) (n^{-1} \mathbb{X}^T \mathbb{X})^{-1} (n^{-1} \mathbb{X}^T \varepsilon) \right\}. \end{aligned}$$

The center term converges to $\Sigma_X > 0$ and the left and right terms converge to 0 a.s. by Lemma 3. Our result follows. \square

Lemma 5. $d_2^r(\widehat{F}_n, F_n) \rightarrow 0$ a.s. and $d_2^r(\widehat{F}_n, F) \rightarrow 0$ a.s.

Proof. From the arguments in the proofs of Lemmas 1 and 2 we have that

$$\begin{aligned} d_2^r(\widehat{F}_n, F_n) &= d_2^r(\widetilde{F}_n, F_n)^2 - \|E(\widetilde{F}_n) - E(F_n)\|^2 + \|E(F_n)\|^2 \\ &= \|n^{-1} \sum_{i=1}^n \varepsilon_i\|^2 - \|n^{-1} \sum_{i=1}^n (\widehat{\varepsilon}_i - \varepsilon_i)\|^2 + d_2^r(\widetilde{F}_n, F_n) \\ &\leq \|n^{-1} \sum_{i=1}^n \varepsilon_i\|^2 + n^{-1} \operatorname{tr} \{(\widehat{\varepsilon} - \varepsilon)^T(\widehat{\varepsilon} - \varepsilon)\} \end{aligned}$$

which converges to 0 a.s. by Lemma 4. Therefore the first convergence result holds. From the metric properties of the Mallows metric we have that

$$\frac{1}{2} d_2^r(\widehat{F}_n, F)^2 \leq d_2^r(\widehat{F}_n, F_n)^2 + d_2^r(F_n, F)^2.$$

Our second convergence result follows from the first convergence result and Lemma 8.4 of Bickel and Freedman (1981). \square

Lemma 6. Let u_i and v_i , $i = 1, \dots, n$, be $r \times 1$ vectors. Let

$$\bar{u} = n^{-1} \sum_{i=1}^n u_i, \quad \text{and} \quad s_u^2 = n^{-1} \sum_{i=1}^n (u_i - \bar{u})(u_i - \bar{u})^T$$

and similarly for v . Then

$$\|s_u^2 - s_v^2\|_F^2 \leq \|n^{-1} \sum_{i=1}^n (u_i - v_i)(u_i - v_i)^T\|_F^2$$

where $\|\cdot\|_F$ is the Frobenius norm.

Proof. We have

$$\begin{aligned} \|s_u^2 - s_v^2\|_F^2 &= \sum_{j=1}^n \sum_{k=1}^n \left| n^{-1} \sum_{i=1}^n (u_i - \bar{u})_j (u_i - \bar{u})_k^T - n^{-1} \sum_{i=1}^n (v_i - \bar{v})_j (v_i - \bar{v})_k^T \right|^2 \\ &\leq \sum_{j=1}^n \sum_{k=1}^n \left| n^{-1} \sum_{i=1}^n (u_i - v_i)_j (u_i - v_i)_k \right|^2 \\ &= \|n^{-1} \sum_{i=1}^n (u_i - v_i)(u_i - v_i)^T\|_F^2, \end{aligned}$$

where the inequality follows from Freedman (1981, Lemma 2.7). \square

The proof of Theorem 1 is now given. Before this theorem, we define the $\operatorname{vech}(A) \in \mathbb{R}^{p(p+1)/2 \times 1}$ operator to be the function that stacks the unique $p(p+1)/2$ elements of any symmetric matrix $A \in \mathbb{R}^{p \times p}$.

Proof. Exchange \widehat{F}_n for G in Theorem 3 and observe that

$$d_2^{pp} \{ \Psi_n(F), \Psi_n(\widehat{F}_n) \} \leq nr \operatorname{tr} \{ (\mathbb{X}^T \mathbb{X})^{-1} \} d_2^r(F, \widehat{F}_n)^2.$$

From Lemma 5 we know that $d_2^r(F, \widehat{F}_n)^2 \rightarrow 0$ almost everywhere. Our result for part (a) follows since F is mean-zero normal with variance $\Sigma_X^{-1} \otimes \Sigma$. We now show that part (b) holds. First, we need to establish that $\widehat{\Sigma} \rightarrow \Sigma$ almost everywhere. To see this, introduce

$$\Sigma_n = n^{-1} \sum_{i=1}^n \varepsilon_i \varepsilon_i^T - \left(n^{-1} \sum_{i=1}^n \varepsilon_i \right) \left(n^{-1} \sum_{i=1}^n \varepsilon_i \right)^T.$$

Clearly, $\Sigma_n \rightarrow \Sigma$ a.s. Let $C_n = n^{-1} \sum_{i=1}^n (\hat{\varepsilon}_i - \varepsilon_i) (\hat{\varepsilon}_i - \varepsilon_i)^T$. We have,

$$\begin{aligned} \|\widehat{\Sigma} - \Sigma_n\|_F^2 &\leq \|C_n\|_F^2 = \text{tr}(C_n C_n) \leq \text{tr}^2(C_n) \\ &= \text{tr}^2 \left\{ n^{-1} \sum_{i=1}^n (\hat{\varepsilon}_i - \varepsilon_i)^T (\hat{\varepsilon}_i - \varepsilon_i) \right\} \\ &= \text{tr}^2 \{ n^{-1} (\widehat{\varepsilon} - \varepsilon)^T (\widehat{\varepsilon} - \varepsilon) \} \rightarrow 0 \end{aligned}$$

a.s. where the first inequality follows from [Lemma 6](#) with $\widehat{\Sigma}_n$ and Σ_n taking the place of s_u^2 and s_v^2 respectively, the second inequality follows from the fact that C_n is positive definite a.s., and the convergence follows from [Lemma 4](#).

Let $D_n = E (\|\widehat{\Sigma}_n^* - \Sigma_n^*\|_F \mid Y_1, \dots, Y_n)$. From [Lemma 6](#) and the proof of [Lemma 1](#) we see that,

$$\begin{aligned} D_n &\leq E \left\{ \left\| n^{-1} \sum_{i=1}^n (\widehat{\varepsilon}_i^* - \varepsilon_i^*) (\widehat{\varepsilon}_i^* - \varepsilon_i^*)^T \right\|_F \mid Y_1, \dots, Y_n \right\} \\ &\leq E \left[\text{tr} \{ n^{-1} (\widehat{\varepsilon}^* - \varepsilon^*)^T (\widehat{\varepsilon}^* - \varepsilon^*) \} \mid Y_1, \dots, Y_n \right] \\ &\leq p \text{tr} (\widehat{\Sigma}) / n \end{aligned}$$

where the last inequality follows from the argument that proves [Lemma 1](#) applied to the starred data, and $p \text{tr} (\widehat{\Sigma}) / n \rightarrow 0$ a.s. It remains to show that $\widehat{\Sigma}_n^*$ converges to Σ . Conditional on Y_1, \dots, Y_n ,

$$\begin{aligned} d_2^{r(r+1)/2} \left\{ n^{-1} \sum_{i=1}^n \text{vech}(\varepsilon_i^* \varepsilon_i^{*T}), n^{-1} \sum_{i=1}^n \text{vech}(\varepsilon_i \varepsilon_i^T) \right\} \\ \leq d_2^{r(r+1)/2} \left\{ \text{vech}(\varepsilon_1^* \varepsilon_1^{*T}), \text{vech}(\varepsilon_1 \varepsilon_1^T) \right\} \end{aligned} \quad (6)$$

by [Lemma 8.6](#) in [Bickel and Freedman \(1981\)](#). Now ε^* has conditional distribution \widehat{F}_n and ε has law F and [Lemma 5](#) gives $d_2^r(\widehat{F}_n, F) \rightarrow 0$ almost everywhere. We now show that $d_1 \left\{ \text{vech}(\varepsilon_1^* \varepsilon_1^{*T}), \text{vech}(\varepsilon_1 \varepsilon_1^T) \right\} \rightarrow 0$ a.s. by [Lemma 8.5](#) of [Bickel and Freedman \(1981\)](#) with $\phi(x) = \text{vech}(xx^T)$ where $x \in \mathbb{R}^r$. To do this, we show that K can be chosen so that $\|\phi(x)\|_1 \leq K(1 + \|x\|_2^2)$ where $\|\cdot\|_1$ and $\|\cdot\|_2$ are the \mathcal{L}^1 and \mathcal{L}^2 norms respectively. From the definition of the Euclidean norm, we have $\|x\|_2^2 = \sum_{i=1}^r x_i^2$. It is clear that $x_i^2 + x_j^2 \geq 2|x_i x_j|$ for all $i, j = 1, \dots, r$. Now, pick $K = \binom{r}{2} + 1$. We see that

$$\begin{aligned} K(1 + \|x\|_2^2) &\geq \left| \sum_{i=1}^r x_i^2 + \binom{r}{2} \sum_{i=1}^r x_i^2 \right| \geq \left| \sum_{i=1}^r x_i^2 + \sum_{i \neq j} |x_i x_j| \right| \\ &\geq \left| \sum_{i \geq j} |x_i x_j| \right| \geq \|\text{vech}(xx^T)\|_1 = \|\phi(x)\|_1. \end{aligned}$$

A similar argument shows that $1/n \sum_{i=1}^n \varepsilon_i^*$ converges to 0. Part (c) follows from both (a) and (b). \square

4.2. Random design and heteroskedasticity

In this section we provide the proof of [Theorem 2](#). Several quantities and lemmas are introduced in order to prove [Theorem 2](#). The logic follows that of [Freedman \(1981, Section 3\)](#). Define,

$$\begin{aligned} \Sigma(\mu) &= \int xx^T \mu(dx), \\ \beta(\mu) &= \int yx^T \mu(dx, dy) \Sigma(\mu)^{-1}, \\ \varepsilon(\mu, x, y) &= y - \beta(\mu)x^T. \end{aligned}$$

The next two lemmas are needed to prove [Theorem 2](#).

Lemma 7. If $d_4^{p+r}(\mu_n, \mu) \rightarrow 0$ as $n \rightarrow \infty$, then

- $\Sigma(\mu_n) \rightarrow \Sigma(\mu)$ and $\beta(\mu_n) \rightarrow \beta(\mu)$,
- the μ_n -law of $\text{vec}\{\varepsilon(\mu_n, x, y)x^T\}$ converges to the μ -law of $\text{vec}\{\varepsilon(\mu, x, y)x^T\}$ in d_2^p ,
- the μ_n -law of $\|\varepsilon(\mu_n, x, y)\|^2$ converges to the μ -law of $\|\varepsilon(\mu, x, y)\|^2$ in d_1 .

Proof. Part (a) immediately follows from [Bickel and Freedman \(1981, Lemma 8.3c\)](#).

We use (Bickel and Freedman, 1981, Lemma 8.3a) to verify part (b). The weak convergence step is evident. Now,

$$\begin{aligned}\|\text{vec}\{\varepsilon(\mu_n, x, y)x^T\}\|^2 &= \|\text{vec}\{yx^T - \beta(\mu_n)xx^T\}\|^2 \\ &= \|\text{vec}(yx^T)\|^2 + \|\text{vec}(\beta(\mu_n)xx^T)\|^2 - 2\text{vec}(yx^T)^T \text{vec}(\beta(\mu_n)xx^T).\end{aligned}$$

Let $z = (x^T, y^T)^T$. Part (b) follows from, integration with respect to μ_n , part (a), and Bickel and Freedman (1981, Lemma 8.5) with $\phi(z) = \text{vech}(zz^T)$. The steps involving (Bickel and Freedman, 1981, Lemma 8.5) are similar to those in the proof of Theorem 1.

Part (c) follows from the same argument used to prove part (b). \square

Lemma 8. $d_4^{p+r}(\mu_n, \mu) \rightarrow 0$ a.e. as $n \rightarrow \infty$.

Proof. The steps are the same as those in Freedman (1981, Lemma 3.2). \square

The proof of Theorem 2 is now given.

Proof. We can write

$$\begin{aligned}\text{vec}\left\{\sqrt{n}\left(\hat{\beta}^* - \hat{\beta}\right)\right\} &= \text{vec}\left[\sqrt{n}\left\{Y^{*T}X^*(X^{*T}X^*)^{-1} - \hat{\beta}\right\}\right] \\ &= \text{vec}\left[\sqrt{n}\left\{(\varepsilon^* + X^*\hat{\beta}^T)^T X^*(X^{*T}X^*)^{-1} - \hat{\beta}\right\}\right] \\ &= \text{vec}\left\{n^{-1/2}\varepsilon^{*T}X^*(n^{-1}X^{*T}X^*)^{-1}\right\} \\ &= \text{vec}\left(Z^*W^{*-1}\right) = \left(W^{*-1} \otimes I_r\right)\text{vec}(Z^*)\end{aligned}$$

where $Z^* = n^{-1/2}\varepsilon^{*T}X^*$ and $W^* = n^{-1}X^{*T}X^*$. Freedman (1981, Theorem 3.1) implies that the conditional law, conditional on $(X_i, Y_i), i = 1, \dots, n$, of $W^* \rightarrow_p \Sigma_X$. This verifies part (a).

We now verify part (b). From Bickel and Freedman (1981, Lemma 8.7), we have

$$d_2^p\{\text{vec}(Z^*), \text{vec}(Z)\}^2 \leq d_2^p\left\{\text{vec}(X_i^* \varepsilon_i^{*T}), \text{vec}(X_i \varepsilon_i^T)\right\}^2$$

where the right side goes to 0 a.e. as $n \rightarrow \infty$. Lemma 8 states that $\mu_n \rightarrow \mu$ a.e. in d_4^{r+p} as $n \rightarrow \infty$ and part (b) of Lemma 7 implies that the distribution of $\text{vec}(Z^*)$, conditional on $(X_i, Y_i), i = 1, \dots, n$, converges to $\text{vec}(Z)$. The random variable $\text{vec}(Z)$ is normally distributed with mean 0 and variance matrix M . Combining this with part (a) verifies that the conditional distribution of $(W^{*-1} \otimes I_r)\text{vec}(Z^*)$ converges to $(\Sigma_X^{-1} \otimes I_r)\text{vec}(Z)$ as $n \rightarrow \infty$. This completes the proof of part (b).

Part (c) follows from the same argument in the proof of Theorem 1 where Lemmas 8 and 7(c) combine to show that (6) converges to 0 as $n \rightarrow \infty$. Note that $\varepsilon_1^* = Y_1^* - \hat{\beta}X_1^*$ in this argument. This completes the proof. \square

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References

- Bickel, P.J., Freedman, D.A., 1981. Some asymptotic theory for the bootstrap. *Ann. Statist.* 9, 1196–1217.
 Chatterjee, S., Bose, A., 2000. Variance estimation in high dimensional models. *Statist. Sinica* 10, 497–515.
 Diaconis, P., Efron, B., 1983. Computer intensive methods in statistics. *Sci. Am.* 248.
 Freedman, D.A., 1981. Bootstrapping regression models. *Ann. Statist.* 9, 1218–1228.
 Freedman, D.A., Peters, S.C., 1984. Bootstrapping a regression equation: some empirical results. *J. Amer. Statist. Assoc.* 79, 97–106.
 Henderson, H.V., Velleman, P.F., 1981. Building multiple regression models interactively. *Biometrics* 37, 391–411.
 Lai, T., Robbins, H., Wei, V., 1979. Strong Consistency of least squares estimated in multiple regression. *J. Multivariate Anal.* 9, 343–361.
 Weisberg, S., 2005. *Applied Linear Regression*. Wiley, New Jersey.