Queen's Economics Department Working Paper No. 1485

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4-2022 (minor revisions)

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April 22, 2022

Abstract

We provide new and computationally attractive methods, based on jackknifing by cluster, to obtain cluster-robust variance matrix estimators (CRVEs) for linear regression models estimated by least squares. These estimators have previously been computationally infeasible except for small samples. We also propose several new variants of the wild cluster bootstrap, which involve the new CRVEs, jackknife-based bootstrap data-generating processes, or both. Extensive simulation experiments suggest that the new methods can provide much more reliable inferences than existing ones in cases where the latter are not trustworthy, such as when the number of clusters is small and/or cluster sizes vary substantially.

Keywords: bootstrap, clustered data, grouped data, cluster-robust variance estimator, CRVE, cluster sizes, jackknife, wild cluster bootstrap

JEL Codes: C10, C12, C21, C23.

*We are grateful to David Drukker, David Roodman, and participants at New York Camp Econometrics 2022 for helpful comments and suggestions. MacKinnon and Webb thank the Social Sciences and Humanities Research Council of Canada (SSHRC grants 435-2016-0871 and 435-2021-0396) for financial support. Nielsen thanks the Danish National Research Foundation for funding a DNRF Chair grant.

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1 Introduction

In applications of linear regression models to many fields of economics and other disciplines, it is common to divide the sample into disjoint clusters and employ a cluster-robust variance matrix estimator (or CRVE) for inference. These estimators are based on the assumption that the disturbances of the regression model are uncorrelated across clusters, but they allow for arbitrary patterns of dependence and heteroskedasticity within each cluster. The literature on cluster-robust inference has grown rapidly in recent years. Cameron and Miller (2015) is a classic survey article. Conley, Gonçalves and Hansen (2018) surveys a broader class of methods for dependent data. MacKinnon, Nielsen and Webb (2022a) provides a guide that explores the implications of key theoretical results for empirical practice, with an emphasis on bootstrap methods.

There are several CRVEs for ordinary least squares (OLS) estimates of linear regression models; see Section 2. However, mainly for computational reasons, almost all empirical work to date has made use of the simplest one, which is usually known as CV_1 and is the default in Stata. Cluster-robust tests and confidence intervals based on CV_1 may or may not yield reliable inferences. Whether they do so depends primarily on the number of clusters G and how homogeneous these are. When all clusters are roughly equal in size and approximately balanced, asymptotic inference based on CV_1 seems to be fairly reliable whenever G is at least moderately large (say 50 or more). However, there are at least two situations in which cluster-robust t-tests and Wald tests are at risk of severe over-rejection, and cluster-robust confidence intervals are at risk of severe under-coverage, even when G is very large. The first is when one or a few clusters are much larger than the rest, and the second is when the only "treated" observations belong to just a few clusters; Djogbenou, MacKinnon and Nielsen (2019) discusses the first case, and MacKinnon and Webb (2017, 2018) discuss the second.

Alternatives to CV_1 have been known since Bell and McCaffrey (2002), but computational difficulties have kept them from widespread use. As we discuss in Section 3, however, recent developments have made it much faster to compute CRVEs based on the cluster jackknife, notably the one known as CV_3, even for large samples. This makes it interesting to compare the finite-sample performance of t-tests based on CV_1 with those of similar procedures based on CV_3. We do this in Sections 6 and 7.

Bootstrap tests are often more reliable in finite samples than asymptotic tests. The best existing procedure seems to be the wild cluster restricted (or WCR) bootstrap proposed in Cameron, Gelbach and Miller (2008). There is also a closely related procedure called the wild cluster unrestricted (or WCU) bootstrap, which generally does not work quite as well. The asymptotic validity of these procedures is proved in Djogbenou et al. (2019),

which also considers their higher-order asymptotic properties. Until a few years ago, the WCR and WCU bootstraps were computationally expensive for large samples, but that is no longer the case. Roodman, MacKinnon, Nielsen and Webb (2019) describes a remarkably efficient implementation in the Stata package `boottest`, and MacKinnon (2022) discusses other methods for fast computation. The `boottest` routines are now available as a `Julia` package which can be also be called from `R`, `Python`, and `Stata`.

The next section establishes notation and briefly reviews the literature on asymptotic cluster-robust inference for the linear regression model, including two well-known alternatives to CV_1, which are often called CV_2 and CV_3. Then Section 3 provides a new computational method for CV_3, which is conceptually simple and, in many cases, extremely fast, as we demonstrate in Section 4.

Section 5 discusses several ways of modifying the wild cluster bootstrap. One modification simply replaces CV_1 by CV_3. The other involves modifying the bootstrap data-generating process, or DGP. Modern treatments of the wild cluster bootstrap, such as MacKinnon et al. (2022a) and MacKinnon (2022), express the bootstrap DGP as a function of the empirical scores. We show how to make the bootstrap DGP more closely resemble the (unknown) true one by transforming the residuals before forming the scores. The transformation we propose is based on the jackknife. Accordingly, it does not actually require any calculations that explicitly involve residuals. This makes it very fast when the number of clusters is small relative to the sample size, even when the latter is extremely large.

Simulation results in Sections 6 and 7 suggest that our new versions of the WCR and WCU bootstraps perform better, and sometimes much better, than the original ones. This is particularly true when cluster sizes vary greatly. Section 8 presents an empirical illustration in which our methods are likely to be more reliable than existing ones, and Section 9 concludes.

2 The Linear Regression Model with Clustering

Consider the linear regression model $y_i = \boldsymbol{x}_i^\top \boldsymbol{\beta} + u_i$. If we divide the data into G disjoint clusters, where the allocation of observations to clusters is assumed to be known, this can be written as

$$\boldsymbol{y}_g = \boldsymbol{X}_g \boldsymbol{\beta} + \boldsymbol{u}_g, \quad g = 1, \dots, G. \tag{1}$$

The g^{th} cluster has N_g observations, and the total sample size is $N = \sum_{g=1}^{G} N_g$. In (1), $\boldsymbol{X}_g$ is an $N_g \times k$ matrix of regressors, $\boldsymbol{\beta}$ is a k-vector of coefficients, $\boldsymbol{y}_g$ is an N_g-vector of observations on the regressand, and $\boldsymbol{u}_g$ is an N_g-vector of disturbances (or error terms). Stacking the $\boldsymbol{y}_g$ yields the N-vector $\boldsymbol{y}$, stacking the $\boldsymbol{X}_g$ yields the $N \times k$ matrix $\boldsymbol{X}$, and stacking the $\boldsymbol{u}_g$ yields the N-vector $\boldsymbol{u}$, so that (1) can be rewritten as $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{u}$.

The OLS estimator of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y} = \boldsymbol{\beta}_0 + (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{u}, \tag{2}$$

where the second equality depends on the assumption that the data are actually generated by (1) with true value $\boldsymbol{\beta}_0$. Thus, if $\boldsymbol{s}_g = \boldsymbol{X}_g^\top \boldsymbol{u}_g$ is the score vector for the g^{th} cluster,

$$\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0 = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \sum_{g=1}^{G} \boldsymbol{X}_g^\top \boldsymbol{u}_g = \Big(\sum_{g=1}^{G} \boldsymbol{X}_g^\top \boldsymbol{X}_g \Big)^{-1} \sum_{g=1}^{G} \boldsymbol{s}_g. \tag{3}$$

Obtaining valid inferences evidently requires assumptions about the score vectors. For a correctly specified model, $\mathrm{E}(\boldsymbol{s}_g) = \boldsymbol{0}$ for all g. We further assume that

$$\mathrm{E}(\boldsymbol{s}_g \boldsymbol{s}_g^\top) = \boldsymbol{\Sigma}_g \quad \text{and} \quad \mathrm{E}(\boldsymbol{s}_g \boldsymbol{s}_{g'}^\top) = \boldsymbol{0}, \quad g, g' = 1, \ldots, G, \quad g' \neq g, \tag{4}$$

where $\boldsymbol{\Sigma}_g$ is the symmetric, positive semidefinite variance matrix of the scores for the g^{th} cluster. The second assumption in (4) is crucial. It states that the scores for every cluster are uncorrelated with the scores for every other cluster.

From the rightmost expression in (3), we see that the distribution of $\hat{\boldsymbol{\beta}}$ depends on the disturbance subvectors $\boldsymbol{u}_g$ only through the distribution of the score vectors $\boldsymbol{s}_g$. It follows immediately that an estimator of $\mathrm{Var}(\hat{\boldsymbol{\beta}})$ should be based on the usual sandwich formula,

$$(\boldsymbol{X}^\top \boldsymbol{X})^{-1} \Big(\sum_{g=1}^{G} \boldsymbol{\Sigma}_g \Big) (\boldsymbol{X}^\top \boldsymbol{X})^{-1}. \tag{5}$$

Every cluster-robust variance estimator replaces the $\boldsymbol{\Sigma}_g$ in (5) by functions of the $\boldsymbol{X}_g$ and the residual subvectors $\hat{\boldsymbol{u}}_g$. There is more than one way to do this, and alternative CRVEs employ different approaches.

Since $\boldsymbol{\Sigma}_g$ is the expectation of $\boldsymbol{s}_g \boldsymbol{s}_g^\top$, the simplest approach is just to replace it by $\hat{\boldsymbol{s}}_g \hat{\boldsymbol{s}}_g^\top$, where $\hat{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top \hat{\boldsymbol{u}}_g$ is the empirical score vector for the g^{th} cluster. If in addition we multiply by a correction for degrees of freedom, we obtain

$$\mathrm{CV}_1\text{:} \qquad \hat{\boldsymbol{V}}_1(\hat{\boldsymbol{\beta}}) = \frac{G(N-1)}{(G-1)(N-k)} (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \Big(\sum_{g=1}^{G} \hat{\boldsymbol{s}}_g \hat{\boldsymbol{s}}_g^\top \Big) (\boldsymbol{X}^\top \boldsymbol{X})^{-1}. \tag{6}$$

This is by far the most widely used CRVE in practice, and it is the default in `Stata`. The leading scalar is chosen so that, when $G = N$, $\hat{\boldsymbol{V}}_1(\hat{\boldsymbol{\beta}})$ reduces to the familiar HC_1 estimator (MacKinnon and White 1985) that is robust only to heteroskedasticity of unknown form.

Inference about $\boldsymbol{\beta}$ is typically based on cluster-robust t-statistics and Wald statistics. If β_j denotes the j^{th} element of $\boldsymbol{\beta}$ and β_{0j} is its value under the null hypothesis, then the

appropriate t-statistic is

$$t_j = \frac{\hat{\beta}_j - \beta_{0j}}{\text{se}_1(\hat{\beta}_j)}, \tag{7}$$

where $\hat{\beta}_j$ is the OLS estimate, and $\text{se}_1(\hat{\beta}_j)$ is the square root of the j^{th} diagonal element of $\hat{\boldsymbol{V}}_1(\hat{\boldsymbol{\beta}})$. Under extremely strong assumptions (Bester, Conley and Hansen 2011), it can be shown that t_j asymptotically follows the $t(G-1)$ distribution. Conventional "asymptotic" inference is based on this distribution.

We should expect inferences based on CV_1 to be reliable if the sum of the $\boldsymbol{s}_g$, suitably normalized, is well approximated by a multivariate normal distribution with mean zero, and if the $\boldsymbol{s}_g$ are well approximated by the $\hat{\boldsymbol{s}}_g$. But asymptotic inference can be misleading when either or both of these approximations is poor; see Djogbenou et al. (2019) and MacKinnon et al. (2022a). Whether or not the first approximation is a good one depends on the model and the data, and there is not much the investigator can do about it. But the second approximation can, in principle, be improved by using modified empirical score vectors instead of the $\hat{\boldsymbol{s}}_g$.

Two CRVEs based on this idea, which today are usually known as CV_2 and CV_3, were proposed (under different names) in Bell and McCaffrey (2002). These are the cluster analogs of the heteroskedasticity-consistent variance matrix estimators HC_2 and HC_3. MacKinnon and White (1985) proposed HC_3 based on the jackknife, after discussing (and naming) HC_1 and HC_2. All of these estimators are designed to compensate, in different ways, for the shrinkage and intra-cluster correlation of the residuals induced by least squares.

The CV_2 variance matrix is

$$\text{CV}_2\text{:} \qquad \hat{\boldsymbol{V}}_2(\hat{\boldsymbol{\beta}}) = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \Big(\sum_{g=1}^{G} \grave{\boldsymbol{s}}_g \grave{\boldsymbol{s}}_g^\top \Big) (\boldsymbol{X}^\top \boldsymbol{X})^{-1}, \tag{8}$$

where the modified score vectors $\grave{\boldsymbol{s}}_g$ are defined as

$$\grave{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top \boldsymbol{M}_{gg}^{-1/2} \hat{\boldsymbol{u}}_g. \tag{9}$$

Here $\boldsymbol{M}_{gg} = \mathbf{I}_{N_g} - \boldsymbol{X}_g (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}_g^\top$ is the diagonal block corresponding to the g^{th} cluster of the projection matrix $\boldsymbol{M}_{\boldsymbol{X}}$, which satisfies $\hat{\boldsymbol{u}} = \boldsymbol{M}_{\boldsymbol{X}} \boldsymbol{u}$, and $\boldsymbol{M}_{gg}^{-1/2}$ is the symmetric square root of its inverse. The CV_2 estimator has been recommended in Imbens and Kolesár (2016) and Pustejovsky and Tipton (2018). Both of these papers also provide methods for computing critical values based on t and F distributions with computed degrees of freedom; MacKinnon and Webb (2018) provides some evidence on how well these work.

The CV_3 variance matrix is very similar to CV_2, but, as we explain in Section 3, it is

based on the jackknife. The usual definition is

$$\text{CV}_3: \qquad \hat{\boldsymbol{V}}_3(\hat{\boldsymbol{\beta}}) = \frac{G-1}{G}(\boldsymbol{X}^\top\boldsymbol{X})^{-1}\Big(\sum_{g=1}^{G}\acute{\boldsymbol{s}}_g\acute{\boldsymbol{s}}_g^\top\Big)(\boldsymbol{X}^\top\boldsymbol{X})^{-1}, \tag{10}$$

where now the modified score vectors $\acute{\boldsymbol{s}}_g$ are defined as

$$\acute{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top\boldsymbol{M}_{gg}^{-1}\hat{\boldsymbol{u}}_g. \tag{11}$$

The rescaling factor $(G-1)/G$ in (10) is the analog of the factor $(N-1)/N$ that occurs in jackknife variance matrix estimators at the individual level. It compensates for the tendency of the jackknife estimates to be too spread out. This factor implicitly assumes that all clusters are the same size and perfectly balanced, with disturbances that are independent and homoskedastic; an alternative rescaling factor based on weaker assumptions is proposed in Niccodemi and Wansbeek (2022).

Although (8) and (10) look simple enough, computing either CV_2 or CV_3 has until recently been extremely expensive, or even computationally infeasible, when any of the N_g are large. The problem is that, before computing (11), we apparently need to rescale the residual vector $\hat{\boldsymbol{u}}_g$ for each cluster. This involves storing and inverting the $N_g \times N_g$ matrix $\boldsymbol{M}_{gg}$. Before computing (9), we also need to compute the symmetric square roots of the $\boldsymbol{M}_{gg}$, and this requires calculating their eigenvalues and eigenvectors. Of course, when all clusters are very small, this is not difficult. When $G = N$, CV_2 reduces to HC_2, and CV_3 reduces to HC_3, both of which can be computed very quickly.

Niccodemi et al. (2020) has recently proposed a method that is much faster for large clusters. Versions of this method apply to both CV_2 and CV_3. Instead of rescaling the residual vectors, it calculates the score vectors $\grave{\boldsymbol{s}}_g$ or $\acute{\boldsymbol{s}}_g$ directly using equations that do not involve any $N_g \times N_g$ matrices. A modified version of this method, which appears to be new, works as follows. First, form the $k \times k$ matrices

$$\boldsymbol{A}_g = (\boldsymbol{X}^\top\boldsymbol{X})^{-1/2}\boldsymbol{X}_g^\top\boldsymbol{X}_g(\boldsymbol{X}^\top\boldsymbol{X})^{-1/2}, \quad g = 1, \dots, G. \tag{12}$$

Then, for (8), calculate the rescaled score vectors

$$\grave{\boldsymbol{s}}_g = (\boldsymbol{X}^\top\boldsymbol{X})^{1/2}(\mathbf{I}_k - \boldsymbol{A}_g)^{-1/2}(\boldsymbol{X}^\top\boldsymbol{X})^{-1/2}\hat{\boldsymbol{s}}_g, \quad g = 1, \dots, G, \tag{13}$$

and, for (10), calculate the rescaled score vectors

$$\acute{\boldsymbol{s}}_g = (\boldsymbol{X}^\top\boldsymbol{X})^{1/2}(\mathbf{I}_k - \boldsymbol{A}_g)^{-1}(\boldsymbol{X}^\top\boldsymbol{X})^{-1/2}\hat{\boldsymbol{s}}_g, \quad g = 1, \dots, G. \tag{14}$$

These rescaled score vectors are used in (8) and (10) as before. Unless all the clusters are very small, computing CV_2 and CV_3 using (13) and (14) is much faster than computing them using (9) and (11); see Section 4.

In the case of CV_3, however, an even faster and more intuitive method is available. This jackknife-based method, which we introduce in the next section, can be extremely fast when N is large and G is much smaller than N, so that at least some clusters are large; see Section 4.

3 Jackknife Variance Matrix Estimators

The jackknife is a simple method for reducing bias and estimating standard errors by omitting observations sequentially. Tukey (1958) suggested using the jackknife to estimate standard errors, and Miller (1974) is a classic reference. In this section, we propose efficient methods, based on the cluster jackknife, for computing two closely related CRVEs. Unless all clusters are extremely small, these methods are faster than the ones discussed in the preceding section. The key idea of the cluster jackknife is to compute G sets of parameter estimates, each of which omits one cluster at a time.

The OLS estimates of $\boldsymbol{\beta}$ when each cluster is omitted in turn are

$$\hat{\boldsymbol{\beta}}^{(g)} = (\boldsymbol{X}^\top\boldsymbol{X} - \boldsymbol{X}_g^\top\boldsymbol{X}_g)^{-1}(\boldsymbol{X}^\top\boldsymbol{y} - \boldsymbol{X}_g^\top\boldsymbol{y}_g), \quad g = 1, \ldots, G. \tag{15}$$

In MacKinnon, Nielsen and Webb (2022b), it is recommended that investigators should routinely calculate the $\hat{\boldsymbol{\beta}}^{(g)}$ and examine them, perhaps using graphical methods. When $\hat{\boldsymbol{\beta}}^{(h)}$ differs greatly from $\hat{\boldsymbol{\beta}}$ for one or more coefficients of interest, it is evident that cluster h is highly influential. On the other hand, when the $\hat{\boldsymbol{\beta}}^{(g)}$ do not vary much across the omitted clusters, no individual cluster is influential.

It is easy to obtain the $\hat{\boldsymbol{\beta}}^{(g)}$ in a computationally efficient manner. We start by calculating the cluster-level matrices and vectors

$$\boldsymbol{X}_g^\top\boldsymbol{X}_g \quad \text{and} \quad \boldsymbol{X}_g^\top\boldsymbol{y}_g, \quad g = 1, \ldots, G. \tag{16}$$

Unless G is very large, this involves very little cost beyond that of computing $\hat{\boldsymbol{\beta}}$, because we can use the quantities in (16) to construct $\boldsymbol{X}^\top\boldsymbol{X}$ and $\boldsymbol{X}^\top\boldsymbol{y}$ and then use (2) to compute $\hat{\boldsymbol{\beta}}$. For typical values of k, it should then be reasonably inexpensive to compute $\hat{\boldsymbol{\beta}}^{(g)}$ for every cluster using (15). The main cost, beyond that of computing $\hat{\boldsymbol{\beta}}$, is that we need to calculate the inverse (or possibly the generalized inverse) of a $k \times k$ matrix for each of the $\hat{\boldsymbol{\beta}}^{(g)}$.

The cluster jackknife estimator of $\text{Var}(\hat{\boldsymbol{\beta}})$ is the cluster analog of the usual jackknife

variance matrix estimator given in Efron (1981), among others. It is defined as

$$\text{CV}_{3\text{J}}: \qquad \hat{\boldsymbol{V}}_{3\text{J}}(\hat{\boldsymbol{\beta}}) = \frac{G-1}{G}\sum_{g=1}^{G}(\hat{\boldsymbol{\beta}}^{(g)} - \bar{\boldsymbol{\beta}})(\hat{\boldsymbol{\beta}}^{(g)} - \bar{\boldsymbol{\beta}})^{\top}, \tag{17}$$

where $\bar{\boldsymbol{\beta}} = G^{-1}\sum_{g=1}^{G}\hat{\boldsymbol{\beta}}^{(g)}$ is the sample average of the $\hat{\boldsymbol{\beta}}^{(g)}$. A special case of this estimator with $G = N$ was applied to linear regression models with independent, heteroskedastic disturbances in MacKinnon and White (1985) and called HC_3. Notice that (17) calculates the variance matrix around $\bar{\boldsymbol{\beta}}$. Centering around $\bar{\boldsymbol{\beta}}$ is common in jackknife variance estimation, but it is also common to center around $\hat{\boldsymbol{\beta}}$, as in Bell and McCaffrey (2002).

There is a very close relationship between $\hat{\boldsymbol{V}}_{3\text{J}}(\hat{\boldsymbol{\beta}})$ and $\hat{\boldsymbol{V}}_{3}(\hat{\boldsymbol{\beta}})$. In fact,

$$\hat{\boldsymbol{V}}_{3}(\hat{\boldsymbol{\beta}}) = \frac{G-1}{G}\sum_{g=1}^{G}(\hat{\boldsymbol{\beta}}^{(g)} - \hat{\boldsymbol{\beta}})(\hat{\boldsymbol{\beta}}^{(g)} - \hat{\boldsymbol{\beta}})^{\top}, \tag{18}$$

which is just (17) with $\bar{\boldsymbol{\beta}}$ replaced by $\hat{\boldsymbol{\beta}}$. This follows from (10) and (11) because

$$(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\acute{\boldsymbol{s}}_g = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{M}_{gg}^{-1}\hat{\boldsymbol{u}}_g = \hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}^{(g)}. \tag{19}$$

Note that the summation in (18) is unchanged if $\hat{\boldsymbol{\beta}}^{(g)} - \hat{\boldsymbol{\beta}}$ is replaced by $\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}^{(g)}$.

Although the second equality in (19) is not new, it will turn out to be very useful in Section 5, and so we now prove it. The middle expression in (19) can be written as

$$(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{M}_{gg}^{-1}\boldsymbol{y}_g - (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{M}_{gg}^{-1}\boldsymbol{X}_g(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}\boldsymbol{y}. \tag{20}$$

Using the updating formula

$$(\boldsymbol{X}^{\top}\boldsymbol{X} - \boldsymbol{X}_g^{\top}\boldsymbol{X}_g)^{-1} = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1} + (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{M}_{gg}^{-1}\boldsymbol{X}_g(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}, \tag{21}$$

$\hat{\boldsymbol{\beta}}^{(g)}$ can be written as the sum of four terms, the first of which is just $\hat{\boldsymbol{\beta}}$. Thus the right-hand side of (19) can be written as

$$\begin{aligned}(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{M}_{gg}^{-1}\boldsymbol{X}_g(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{y}_g + (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{y}_g \\ - (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{M}_{gg}^{-1}\boldsymbol{X}_g(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}\boldsymbol{y}.\end{aligned} \tag{22}$$

The last term in (22) is identical to the last term in (20). The first two terms in (22) can be rewritten as

$$(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{M}_{gg}^{-1}\boldsymbol{P}_{gg}\boldsymbol{y}_g + (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}\boldsymbol{y}_g,$$

where $\boldsymbol{P}_{gg} = \boldsymbol{X}_g(\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}_g^{\top}$ is the g^{th} diagonal block of the matrix $\boldsymbol{P}_{\boldsymbol{X}} = \mathbf{I} - \boldsymbol{M}_{\boldsymbol{X}}$; that

is, $\boldsymbol{P}_{gg} = \mathbf{I} - \boldsymbol{M}_{gg}$. Inserting this straightforwardly yields the result that

$$\begin{aligned}&(\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}_g^\top\boldsymbol{M}_{gg}^{-1}\boldsymbol{P}_{gg}\boldsymbol{y}_g + (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}_g^\top\boldsymbol{y}_g \\ &\quad = (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}_g^\top\boldsymbol{M}_{gg}^{-1}(\mathbf{I} - \boldsymbol{M}_{gg})\boldsymbol{y}_g + (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}_g^\top\boldsymbol{y}_g = (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}_g^\top\boldsymbol{M}_{gg}^{-1}\boldsymbol{y}_g.\end{aligned} \tag{23}$$

The right-hand side of (23) is the first term in (20), which proves the second equality in (19).

When $N_g = 1$ for all g, $\hat{\boldsymbol{V}}_{3\mathrm{J}}(\hat{\boldsymbol{\beta}})$ is numerically equal to the original HC_3 estimator proposed in MacKinnon and White (1985), which is actually computed in a way similar to (10) and (11), because this is the fastest method when each cluster contains just one observation. The modern version of HC_3, which uses $\hat{\boldsymbol{\beta}}$ instead of $\bar{\boldsymbol{\beta}}$, seems to be due to Davidson and MacKinnon (1993, Chapter 16). For this version, each residual is simply divided by the corresponding diagonal element of $\boldsymbol{M}_{\boldsymbol{X}}$ prior to computing the filling in the sandwich, and the factor of $(N-1)/N$ is usually (but incorrectly) omitted.

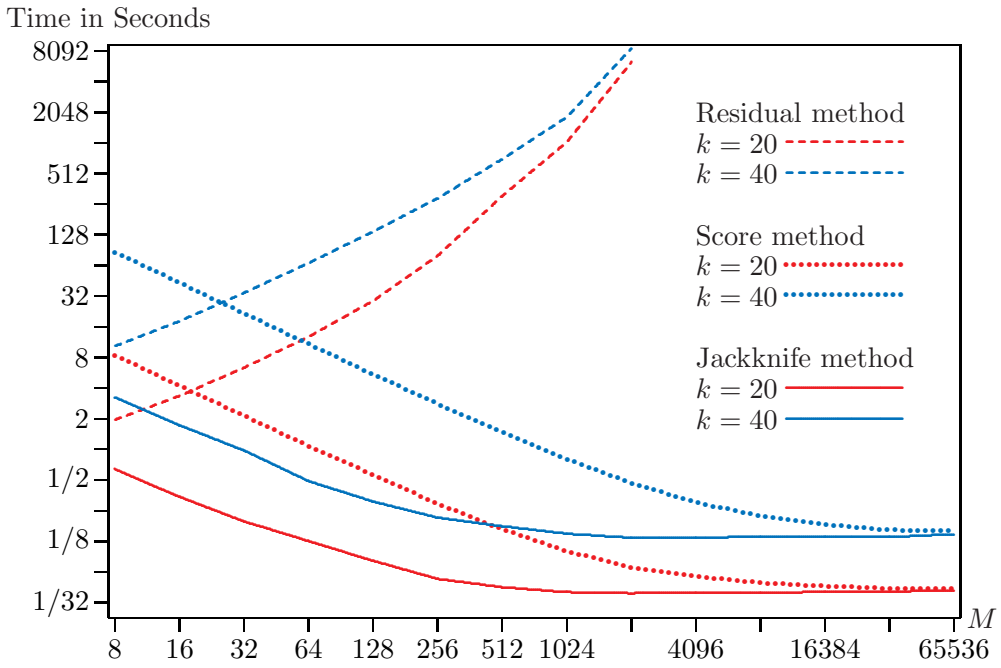
Both cluster jackknife estimators may be used to compute cluster-robust t-statistics. In view of the fact that there are G terms in the summation, it seems natural to compare these with quantiles of the $t(G-1)$ distribution, as usual. These procedures should almost always be more conservative than t-tests based on the widely-used CV_1 estimator. We expect CV_3 and $\mathrm{CV}_{3\mathrm{J}}$ to be very similar in most cases, and there seems to be no good reason to expect either of them to perform better in general. These issues will be investigated in Section 6, where we conclude that it is reasonable to focus on CV_3. MacKinnon et al. (2022b) describes the `Stata` package `summclust`, which calculates CV_3 and $\mathrm{CV}_{3\mathrm{J}}$ for a coefficient of interest. It also calculates a number of summary statistics that may be used to assess the reliability of cluster-robust inference.

4 Speed of Computation

Because the CV_3 estimator has been challenging to compute until recently, it has rarely been used in empirical work. Following Bell and McCaffrey (2002), computation has employed what we call the "residual method" based on (11). To compute the modified score vector $\acute{\boldsymbol{s}}_g$ for the g^{th} cluster, it uses the N_g-vector of residuals $\hat{\boldsymbol{u}}_g$ and the $N_g \times N_g$ matrix $\boldsymbol{M}_{gg}^{-1}$. Unless every N_g is small, storing and inverting the $\boldsymbol{M}_{gg}$ matrices is computationally expensive. Indeed, for even moderately large values of the N_g, this can be effectively impossible, as we demonstrate below.

A much faster method, recently proposed in Niccodemi et al. (2020) and improved slightly in Section 2, uses (14) to obtain the modified score vectors $\acute{\boldsymbol{s}}_g$. Since it operates directly on the score vectors $\hat{\boldsymbol{s}}_g$, we call it the "score method." An even easier approach, proposed in Section 3, computes the $\hat{\boldsymbol{\beta}}^{(g)}$ using (15) and then calculates their variance matrix as (18).

Figure 1: Timings for three ways to compute CV_3



Notes: The sample size is $N = 2^{20} = 1,048,576$. The number of clusters varies from 16 to 131,072. All clusters have $M = N/G$ observations, so that cluster sizes vary from 8 to 65,536. The number of regressors k is either 20 or 40. Times required to compute $\hat{\boldsymbol{\beta}}$ are included; see text. All computations were performed in Fortran using one core of an Intel i9-10850K processor running at 3.6 GHz.

For obvious reasons, we refer to this as the "jackknife method."

In order to compare timings for the residual, score, and jackknife methods, we generate two datasets with $N = 2^{20} = 1,048,576$ observations and G equal-sized clusters, where G varies from 16 to 131,072. Thus the cluster size $M = N/G$ varies from 8 to 65,536. In one case, there are 20 regressors, and in the other case there are 40.

Figure 1 shows the time in seconds, on a $\log_2$ scale, for each of the three methods and the two datasets. These times include the time required to compute the OLS estimates. The residual method requires that $\hat{\boldsymbol{\beta}}$ be computed first, but, for both the score and jackknife methods, intermediate calculations can be used in the computation of $\hat{\boldsymbol{\beta}}$. For large clusters, the cost of computing both the OLS estimates and CV_3 using one or both of these methods was sometimes less than the cost of computing the OLS estimates alone, even though we used a reasonably efficient routine for the latter. This is probably because of cache congestion, which seems to be alleviated by forming $\boldsymbol{X}^\top\boldsymbol{X}$ on a cluster-by-cluster basis. For large clusters, the speed of all methods could almost certainly be increased by using a fast BLAS implementation. However, in the interest of programming ease, we have not done this. The better methods are already very fast.

In Figure 1, the horizontal axis shows cluster sizes $M = N/G$, which vary from 8 to $65,536$. The residual method works well for very small values of M. It is actually faster than the score method for $M = 8$ and $M = 16$. However, its cost rises very rapidly as M increases. The largest value of M for which we were able to compute it was 2048. When $M = 4096$, the program eventually ran out of memory on a machine with 32 GB of RAM. This should have been expected, since storing 256 M_{gg} matrices that are each 4096×4096 requires precisely 32 GB of memory (where each real number uses 8 bytes of storage and a GB is 2^{30} bytes). Of course, the memory limit could have been relaxed substantially by storing only one of the $\boldsymbol{M}_{gg}$ matrices at a time, but it is clear from the figure that using the residual method for $M > 4096$ would have been extremely expensive.

In contrast, both the score and jackknife methods become faster as M increases and G consequently decreases. The jackknife method is always quicker than the score method. For small values of M, it seems to be faster by a factor of about 12 when $k = 20$ and by a factor of about 26 when $k = 40$. However, the advantage of the jackknife method gradually diminishes as M increases. When $M = 65,536$, so that there are only 16 clusters, both methods take almost the same amount of time.

Based on these results, the jackknife method for computing CV_3 is the procedure of choice unless all clusters are tiny (say, $N_g \leq 4$ for all g). For datasets with large clusters, an efficient implementation of this method can compute both the OLS estimates and the CV_3 variance matrix in roughly the same amount of time as a reasonably fast program for the OLS estimates alone.

5 New Versions of the Wild Cluster Bootstrap

The existing version of the WCR bootstrap often, but not always, works well. In this section, we therefore propose three new versions of the WCR bootstrap, along with three corresponding versions of the WCU bootstrap. These are based on two distinct modifications. One involves replacing CV_1 by CV_3. The other involves modifying the bootstrap DGP in a fashion inspired by the modified scores used in the two variance matrices, in the hope that these modified DGPs will provide better approximations to the unknown process that actually generates the data.

We first discuss the bootstrap DGPs for existing versions of the wild cluster bootstrap, expressing them in terms of scores instead of observations. This approach is intuitive and computationally attractive (MacKinnon 2022). The DGP for the wild cluster bootstrap is normally written as a process that generates N observations on a bootstrap dependent

variable y^*. However, in terms of the G score vectors, a generic wild cluster bootstrap DGP is

$$\boldsymbol{s}_g^{*b} = v_g^{*b} \ddot{\boldsymbol{s}}_g, \quad g = 1, \ldots, G, \quad b = 1, \ldots, B, \tag{24}$$

where b indexes bootstrap samples, v_g^{*b} is a random variate with mean 0 and variance 1, and the $\ddot{\boldsymbol{s}}_g$ are empirical score vectors to be discussed below. In most cases, it seems to be best to generate the v_g^{*b} using the Rademacher distribution, which takes the values 1 and -1 with equal probabilities (Davidson and Flachaire 2008; Djogbenou et al. 2019). However, since the number of possible Rademacher bootstrap samples is only $2^G - 1$, it is better to use a distribution with more mass points, such as the six-point distribution proposed in Webb (2014), when G is less than about 12.

The vector $\ddot{\boldsymbol{s}}_g$ in (24) is an empirical score vector for the g^{th} cluster. For the classic WCU bootstrap, it is simply the unrestricted empirical score vector $\hat{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top \hat{\boldsymbol{u}}_g$. For the classic WCR bootstrap, it is the restricted empirical score vector $\tilde{\boldsymbol{s}}_g$ defined as

$$\tilde{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top \boldsymbol{y}_g - \boldsymbol{X}_g^\top \boldsymbol{X}_g \tilde{\boldsymbol{\beta}}, \quad g = 1, \ldots, G, \tag{25}$$

where $\tilde{\boldsymbol{\beta}}$ is the vector of OLS estimates under the null hypothesis. Like $\hat{\boldsymbol{\beta}}$, $\tilde{\boldsymbol{s}}_g$ is a k-vector, even though some elements of $\tilde{\boldsymbol{\beta}}$ may equal zero or satisfy other linear restrictions. The bootstrap DGP (24) looks very much like the one for the wild score cluster bootstrap for nonlinear models proposed in Kline and Santos (2012). In the context of (1), however, it is just a different way of writing the bootstrap DGP for the wild cluster bootstrap.

In order to calculate a bootstrap P value or a bootstrap confidence interval, we need to compute B bootstrap test statistics indexed by b. These depend only on the bootstrap scores in (24) and the matrix $(\boldsymbol{X}^\top \boldsymbol{X})^{-1}$. For each bootstrap sample, we use $\boldsymbol{s}_g^{*b}$ to obtain a bootstrap estimate, not of $\boldsymbol{\beta}$ itself, but of the vector $\boldsymbol{\delta} = \boldsymbol{\beta} - \ddot{\boldsymbol{\beta}}$, where $\ddot{\boldsymbol{\beta}} = \tilde{\boldsymbol{\beta}}$ for the WCR bootstrap and $\ddot{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}$ for the WCU bootstrap. This estimate is simply

$$\hat{\boldsymbol{\delta}}^{*b} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \sum_{g=1}^{G} \boldsymbol{s}_g^{*b} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{s}^{*b}, \tag{26}$$

where $\boldsymbol{s}^{*b} = \sum_{g=1}^{G} \boldsymbol{s}_g^{*b}$. When $v_g^{*b} = 1$ for all g, the bootstrap sample is the same as the original sample. In this very special case, $\hat{\boldsymbol{\delta}}^{*b} = \boldsymbol{0}$ for the WCU bootstrap, and $\hat{\boldsymbol{\delta}}^{*b} = \hat{\boldsymbol{\beta}} - \tilde{\boldsymbol{\beta}}$ for the WCR bootstrap.

A good deal of computer time can be saved by evaluating only one element of $\hat{\boldsymbol{\delta}}^{*b}$. If we are testing the hypothesis that $\beta_j = 0$, where β_j is an element of $\boldsymbol{\beta}$, then we just need to multiply the j^{th} row of $(\boldsymbol{X}^\top \boldsymbol{X})^{-1}$ by $\boldsymbol{s}^{*b}$ in order to obtain $\hat{\delta}_j^{*b}$, the j^{th} element of $\boldsymbol{\delta}^{*b}$. The

bootstrap t-statistic is then equal to

$$t_j^{*b} = \frac{\hat{\delta}_j^{*b}}{\text{se}(\hat{\delta}_j^{*b})}, \tag{27}$$

where $\text{se}(\cdot)$ denotes the standard error formula used to obtain t_j, the original t-statistic. Notice that we automatically get the correct numerator. In this case, it is $\hat{\beta}_j^{*b}$ for the WCR bootstrap, since $\ddot{\boldsymbol{\beta}} = \tilde{\boldsymbol{\beta}}$, and $\hat{\beta}_j^{*b} - \hat{\beta}_j$ for the WCU bootstrap, since $\ddot{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}$. As usual, a symmetric bootstrap P value is then given by

$$P_{\text{S}}^*(t_j) = \frac{1}{B} \sum \mathbb{I}\Big(|t_j^{*b}| > |t_j|\Big), \tag{28}$$

where $\mathbb{I}(\cdot)$ denotes the indicator function. The bootstrap P value in (28) is simply the fraction of the bootstrap samples for which $|t_j^{*b}|$ is more extreme than $|t_j|$. The value of B should be chosen so that $\alpha(B+1)$ is an integer, where α is the level of the test (Racine and MacKinnon 2007). It is common to use $B = 999$ or $B = 9999$.

In the classic version of the wild cluster bootstrap, the standard error formula is $\text{se}_1(\cdot)$, which is based on CV_1. But the results in Section 3 make it equally feasible to use standard errors based on CV_3, even in large samples. This gives us a new version of the WCR bootstrap and a new version of the WCU bootstrap. The bootstrap standard errors can be calculated without computing an entire variance matrix for each bootstrap sample. For example, the CV_3 standard error of $\hat{\delta}_j^{*b}$ is just

$$\text{se}_3(\hat{\delta}_j^{*b}) = \left(\frac{G-1}{G} \sum_{g=1}^{G} \left(\hat{\delta}_{j(g)}^{*b} - \hat{\delta}_j^{*b} \right)^2 \right)^{1/2}, \tag{29}$$

where $\hat{\delta}_{j(g)}^{*b}$ is the j^{th} element of the vector

$$\hat{\boldsymbol{\delta}}_{(g)}^{*b} = (\boldsymbol{X}^\top \boldsymbol{X} - \boldsymbol{X}_g^\top \boldsymbol{X}_g)^{-1} (\boldsymbol{s}^{*b} - \boldsymbol{s}_g^{*b}). \tag{30}$$

Only $\hat{\delta}_j^{*b}$ and the $\hat{\delta}_{j(g)}^{*b}$ need to be computed for each bootstrap sample.

We now have two versions of the WCR bootstrap, which we may refer to as WCR_{11} and WCR_{13}. Here the first subscript identifies the bootstrap DGP as (24) with $\ddot{\boldsymbol{s}}_g = \tilde{\boldsymbol{s}}_g$. The second subscript shows the standard error used to calculate both the actual and bootstrap test statistics to be $\text{se}_1(\cdot)$ or $\text{se}_3(\cdot)$, respectively. Similarly, the two versions of the WCU bootstrap are WCU_{11} and WCU_{13}. The first subscript identifies the bootstrap DGP as (24) with $\ddot{\boldsymbol{s}}_g = \hat{\boldsymbol{s}}_g$, and the second subscript once again indicates the standard error formula.

The WCR_{1x} and WCU_{1x} bootstraps use the restricted or unrestricted empirical scores in their raw form. But empirical scores differ from true scores, because residuals differ from

disturbances. It therefore seems attractive to replace the empirical score vectors for the WCR and WCU bootstraps by modified score vectors that implicitly rescale the residuals on a cluster-by-cluster basis. This is analogous to methods discussed in Davidson and Flachaire (2008) and MacKinnon (2013) for the ordinary wild bootstrap.

We first consider the WCU bootstrap, since this case is slightly easier to deal with. In principle, we could simply replace the vectors $\ddot{\boldsymbol{s}}_g$ in (24) with the modified empirical score vectors $\acute{\boldsymbol{s}}_g$ defined in (11). However, using (11) is expensive, or even computationally infeasible, for large clusters. But the result (19) lets us compute $\acute{\boldsymbol{s}}_g$ very rapidly as

$$\acute{\boldsymbol{s}}_g = \boldsymbol{X}^\top \boldsymbol{X}(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}^{(g)}), \quad g = 1, \ldots, G. \tag{31}$$

For large clusters, using (14) to compute the $\acute{\boldsymbol{s}}_g$ is much faster than using (11), but using (31) is faster still; see Section 4. This yields two new bootstrap methods, WCU_{31} and WCU_{33}, where the initial "3" subscript indicates that we are using $\acute{\boldsymbol{s}}_g$ instead of $\hat{\boldsymbol{s}}_g$. The bootstrap DGP and the standard error formula match for the latter, but not for the former.

It is conceptually straightforward to specify a restricted wild bootstrap DGP based on modified score vectors. Suppose the restrictions have the usual linear form, $\boldsymbol{R}\boldsymbol{\beta} = \boldsymbol{r}$, for a given matrix $\boldsymbol{R}$ and a given vector $\boldsymbol{r}$. We can write this equivalently in terms of free parameters, $\boldsymbol{\phi}$, as $\boldsymbol{\beta} = \boldsymbol{H}\boldsymbol{\phi} + \boldsymbol{h}$ for a given matrix $\boldsymbol{H}$ and a given vector $\boldsymbol{h}$. Then the modified score vectors are

$$\dot{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top \tilde{\boldsymbol{M}}_{gg}^{-1}(\boldsymbol{y}_g - \boldsymbol{X}_g\tilde{\boldsymbol{\beta}}), \tag{32}$$

which are the analogs of the $\acute{\boldsymbol{s}}_g$ from (11). Here $\tilde{\boldsymbol{M}}_{gg}$ is the g^{th} diagonal block of the projection matrix $\tilde{\boldsymbol{M}} = \mathbf{I} - \tilde{\boldsymbol{X}}(\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^\top$, where $\tilde{\boldsymbol{X}} = \boldsymbol{X}\boldsymbol{H}$. However, evaluating (32) is computationally infeasible when the clusters are not all small. We need to replace (32) by something that is feasible for any sample size.

The first step is to compute the restricted estimates $\tilde{\boldsymbol{\beta}} = \boldsymbol{H}\tilde{\boldsymbol{\phi}}+\boldsymbol{h}$ with $\tilde{\boldsymbol{\phi}} = (\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{y}}$ and $\tilde{\boldsymbol{y}} = \boldsymbol{y} - \boldsymbol{X}\boldsymbol{h}$. The corresponding estimates when each cluster is omitted in turn are $\tilde{\boldsymbol{\beta}}^{(g)} = \boldsymbol{H}\tilde{\boldsymbol{\phi}}^{(g)} + \boldsymbol{h}$, where

$$\tilde{\boldsymbol{\phi}}^{(g)} = (\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}} - \tilde{\boldsymbol{X}}_g^\top\tilde{\boldsymbol{X}}_g)^{-1}(\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{y}} - \tilde{\boldsymbol{X}}_g^\top\tilde{\boldsymbol{y}}_g), \quad g = 1, \ldots, G. \tag{33}$$

Then it can be shown that

$$\dot{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top\tilde{\boldsymbol{y}}_g - \boldsymbol{X}_g^\top\tilde{\boldsymbol{X}}_g\tilde{\boldsymbol{\phi}}^{(g)}, \quad g = 1, \ldots, G. \tag{34}$$

To see that (32) and (34) are equal, note that the right-hand side of (34) is

$$\begin{aligned}&\boldsymbol{X}_g^\top\big(\tilde{\boldsymbol{y}}_g - \tilde{\boldsymbol{X}}_g(\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}} - \tilde{\boldsymbol{X}}_g^\top\tilde{\boldsymbol{X}}_g)^{-1}(\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{y}} - \tilde{\boldsymbol{X}}_g^\top\tilde{\boldsymbol{y}}_g)\big)\\ &\quad= \boldsymbol{X}_g^\top\Big(\tilde{\boldsymbol{y}}_g - \tilde{\boldsymbol{X}}_g\Big((\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}})^{-1} + (\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}_g^\top\tilde{\boldsymbol{M}}_{gg}^{-1}\tilde{\boldsymbol{X}}_g(\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}})^{-1}\Big)(\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{y}} - \tilde{\boldsymbol{X}}_g^\top\tilde{\boldsymbol{y}}_g)\Big),\end{aligned}$$

where the equality uses the updating formula (21) applied to $\tilde{\boldsymbol{X}}$, $\tilde{\boldsymbol{X}}_g$, and $\tilde{\boldsymbol{M}}_{gg}^{-1}$. Then we use the fact that $\tilde{\boldsymbol{\phi}} = (\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{y}}$ together with the relation $\tilde{\boldsymbol{X}}_g(\tilde{\boldsymbol{X}}^\top\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}_g^\top = \tilde{\boldsymbol{P}}_{gg} = \mathbf{I} - \tilde{\boldsymbol{M}}_{gg}$ to rewrite the last expression as

$$\begin{aligned}&\boldsymbol{X}_g^\top\big(\tilde{\boldsymbol{y}}_g - \tilde{\boldsymbol{X}}_g\tilde{\boldsymbol{\phi}} - (\mathbf{I} - \tilde{\boldsymbol{M}}_{gg})\tilde{\boldsymbol{M}}_{gg}^{-1}\tilde{\boldsymbol{X}}_g\tilde{\boldsymbol{\phi}} + (\mathbf{I} - \tilde{\boldsymbol{M}}_{gg})\tilde{\boldsymbol{y}}_g + (\mathbf{I} - \tilde{\boldsymbol{M}}_{gg})\tilde{\boldsymbol{M}}_{gg}^{-1}(\mathbf{I} - \tilde{\boldsymbol{M}}_{gg})\tilde{\boldsymbol{y}}_g\big)\\ &\quad= \boldsymbol{X}_g^\top\tilde{\boldsymbol{M}}_{gg}^{-1}(\tilde{\boldsymbol{y}}_g - \tilde{\boldsymbol{X}}_g\tilde{\boldsymbol{\phi}}).\end{aligned} \tag{35}$$

Replacing $\tilde{\boldsymbol{y}}_g$ by $\boldsymbol{y}_g - \boldsymbol{X}_g\boldsymbol{h}$ and $\tilde{\boldsymbol{X}}_g$ by $\boldsymbol{X}_g\boldsymbol{H}$, and using the fact that $\boldsymbol{H}\tilde{\boldsymbol{\phi}} = \tilde{\boldsymbol{\beta}} - \boldsymbol{h}$, the right-hand side of (35) equals (32).

An important special case is the exclusion restriction that $\beta_k = 0$. This is obtained by setting $\boldsymbol{R} = (0, \ldots, 0, 1)$ and $\boldsymbol{r} = 0$, or, equivalently, $\boldsymbol{H} = (\mathbf{I}_{k-1}, \mathbf{0})^\top$ and $\boldsymbol{h} = \mathbf{0}$. In this case we find that $\tilde{\boldsymbol{X}} = \boldsymbol{X}_1$, which contains the first $k-1$ columns of $\boldsymbol{X}$ and $\tilde{\boldsymbol{\phi}} = \tilde{\boldsymbol{\beta}}_1 = (\boldsymbol{X}_1^\top\boldsymbol{X}_1)^{-1}\boldsymbol{X}_1^\top\boldsymbol{y}$. The corresponding estimates when each cluster is omitted in turn are

$$\tilde{\boldsymbol{\beta}}_1^{(g)} = (\boldsymbol{X}_1^\top\boldsymbol{X}_1 - \boldsymbol{X}_{1g}^\top\boldsymbol{X}_{1g})^{-1}(\boldsymbol{X}_1^\top\boldsymbol{y} - \boldsymbol{X}_{1g}^\top\boldsymbol{y}_g), \quad g = 1, \ldots, G,$$

where $\boldsymbol{X}_{1g}$ contains the first $k-1$ columns of $\boldsymbol{X}_g$. Then (34) reduces to

$$\dot{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top\boldsymbol{y}_g - \boldsymbol{X}_g^\top\boldsymbol{X}_{1g}\tilde{\boldsymbol{\beta}}_1^{(g)}, \quad g = 1, \ldots, G.$$

Exactly the same arguments that led to (34) can also be applied to the modified unrestricted empirical scores, giving us

$$\acute{\boldsymbol{s}}_g = \boldsymbol{X}_g^\top\boldsymbol{y}_g - \boldsymbol{X}_g^\top\boldsymbol{X}_g\hat{\boldsymbol{\beta}}^{(g)}, \quad g = 1, \ldots, G. \tag{36}$$

Either (31) or (36) can be used to compute the $\acute{\boldsymbol{s}}_g$, and both are computationally attractive. However, in situations where both $\dot{\boldsymbol{s}}_g$ and $\acute{\boldsymbol{s}}_g$ need to be computed, (36) may offer some programming advantages relative to (31) due to its similarity to (34).

It may seem puzzling that the scalar factors in (6) and (10) do not appear in the bootstrap DGPs that correspond to them. The reason is that rescaling all the bootstrap scores by the same factor has no impact on the resulting bootstrap t-statistics. From (26) and (30), it is easy to see that multiplying all the $\boldsymbol{s}_g^{*b}$ by a scalar C simply makes $\hat{\boldsymbol{\delta}}^{*b}$ and all the $\hat{\boldsymbol{\delta}}_{(g)}^{*b}$ larger by a factor of C. But this also makes the empirical scores for every bootstrap sample larger by the same factor. Therefore, from (6), (8), and (10), the variance matrices become

larger by a factor of C^2 and the standard errors by a factor of C. The factors of C in the numerator and denominator of t_j^{*b} cancel out, leaving the bootstrap t-statistics unchanged.

However, if we chose not to studentize the test statistic, it would make sense to multiply the right-hand side of (24) by the square root of $G(N-1)/((G-1)(N-k))$ in the case of WCU_{1x} and by the square root of $(G-1)/G$ in the case of WCU_{3x}, for $x = 1, 3$. Doing this should improve the correspondence between the bootstrap DGP and the unknown process that actually generated the data. An unstudentized test statistic for $\beta_j = 0$ is just $\hat{\beta}_j$, and its bootstrap analog would be $\hat{\delta}_j^{*b} = \hat{\beta}_j^{*b}$ for the WCR bootstrap and $\hat{\delta}_j^{*b} = \hat{\beta}_j^{*b} - \hat{\beta}_j$ for the WCU bootstrap. The usual theory of higher-order refinements for the bootstrap suggests that it is generally better to studentize (Hall 1992). However, there may be cases in which unstudentized test statistics are of interest (Canay, Santos and Shaikh 2020). Nevertheless, since we will soon have eight bootstrap methods based on t-statistics to study, we do not consider unstudentized statistics further.

It seems highly likely that all the methods discussed in this section are asymptotically valid. That is, under suitable regularity conditions, the rejection frequencies for any test converge to the nominal level of the test as $G \to \infty$. Formal proofs could be obtained by modifying the arguments in Djogbenou et al. (2019). For the WCU bootstrap methods, the key fact is that the modified unrestricted empirical score vectors $\acute{\boldsymbol{s}}_g$ defined in (11) and computed using (31) are asymptotically equal to the ordinary unrestricted empirical score vectors $\hat{\boldsymbol{s}}_g$. For the WCR bootstrap methods, the key fact is that the modified restricted empirical score vectors $\dot{\boldsymbol{s}}_g$ defined in (34) are asymptotically equal to the ordinary restricted empirical score vectors $\tilde{\boldsymbol{s}}_g$ in (25).

6 Simulations: Test Reliability

Previous simulation results in MacKinnon and Webb (2017, 2018), Brewer et al. (2018), Djogbenou et al. (2019), MacKinnon (2022), and several other papers have shown that the reliability of both bootstrap and asymptotic methods for cluster-robust inference depends heavily on the number of clusters, the extent to which cluster sizes vary, and (in the case of treatment effects) both the number of treated clusters and their sizes. Many of our experiments therefore focus on these features.

The model we consider is

$$y_{gi} = \beta_1 + \sum_{j=2}^{k} \beta_j X_{jgi} + u_{gi}, \quad g = 1, \ldots, G, \quad i = 1, \ldots, N_g, \tag{37}$$

where the u_{gi} are generated by a normal random-effects model with intra-cluster correla-

tion ρ. The way in which the $k-1$ non-constant regressors are generated varies across the experiments. The hypothesis to be tested is that $\beta_k = 0$.

In most of our experiments, there are $N = 400G$ observations, which are divided among the G clusters using the formula

$$N_g = \left[N \frac{\exp(\gamma g/G)}{\sum_{j=1}^{G} \exp(\gamma j/G)} \right], \quad g = 1, \ldots, G-1, \tag{38}$$

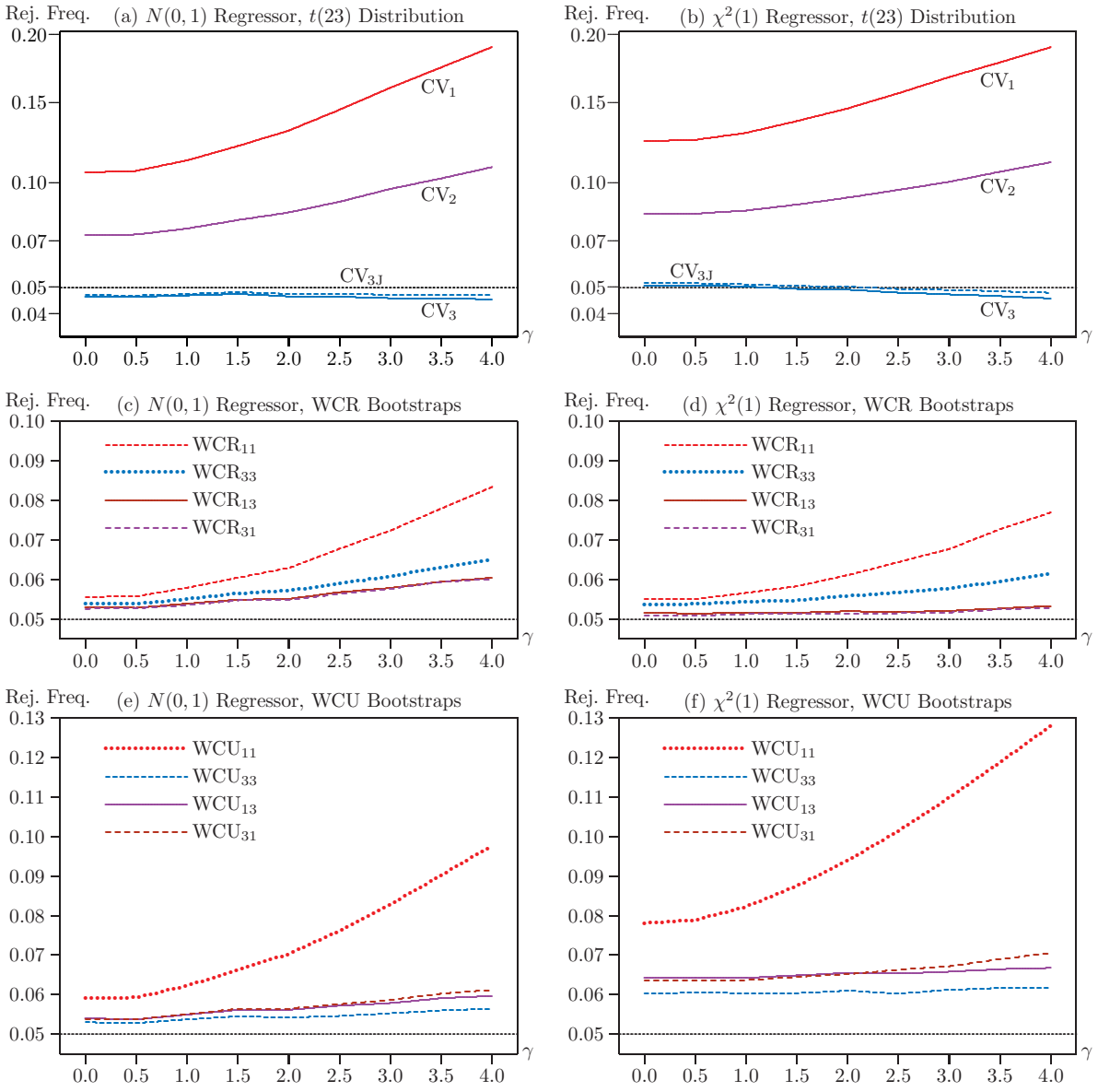
where $[x]$ means the integer part of x. The value of N_G is then set to $N - \sum_{g=1}^{G-1} N_g$. The key parameter here is γ, which determines how uneven the cluster sizes are. When $\gamma = 0$ and N/G is an integer, (38) implies that $N_g = N/G$ for all g. For $\gamma > 0$, cluster sizes vary more and more as γ increases. The largest value of γ that we use is 4. In that case, when $G = 24$ and $N = 9600$, the largest cluster (1513 observations) is about 47 times as large as the smallest cluster (32 observations). When $\gamma = 2$, the variation in cluster sizes is much more moderate. The largest cluster (899 observations) is just under seven times as large as the smallest (130 observations).

The sample sizes that we employ are unusually large for experiments of this type. Since cluster-robust inference is often used with samples that have hundreds of thousands or even millions of observations, we want our results to apply to such cases. In preliminary experiments, we found that the results tended to change slightly, but systematically, as small values of N/G were increased. The results for $N/G > 400$ are very similar to ones for $N/G = 400$, so we use 400 in all the experiments based on (38). Because the bootstrap samples are generated using scores, the cost of the experiments increases much less than proportionally with N/G.

All experiments use $400,000$ replications. This number is so large that experimental randomness is usually negligible. The most important determinant of computational cost is k, the number of regressors. As can be seen from (24) and (34) or (36), generating each bootstrap sample involves $O(k^2 G)$ operations. So does calculating the test statistics using either CV_1 or CV_3. Thus the experiments can be somewhat costly when k is large. Nevertheless, many of our experiments involve $k \geq 10$. We do this because results in MacKinnon (2022) suggest that the performance of many methods of inference deteriorates as k increases. Previous Monte Carlo experiments, which often use $k \leq 3$, may therefore have tended to give too optimistic a picture.

It might seem that substantial savings could be achieved by partialing out all regressors except the one(s) of interest prior to performing the bootstrap. However, this trick does not work. For methods based on the jackknife, it is easy to see why not. If we were to partial out some of the regressors prior to computing the delete-one-cluster estimates in (15), then the computed $\hat{\boldsymbol{\beta}}^{(g)}$ would depend on the values of the partialed-out regressors for the full sample,

Figure 2: Rejection frequencies as a function of γ



Notes: The vertical axes show rejection frequencies for tests of $\beta_k = 0$ in (37) at the .05 level. Results are based on 400,000 replications, with $B = 399$ bootstrap samples. There are 24 clusters, 9600 observations, and 10 regressors, with $\rho = 0.10$. The extent to which cluster sizes vary increases with γ; see (38).

including those in the g^{th} cluster, which would be incorrect. Consequently, the values of the delete-one-cluster estimates will be incorrect if we partial out any regressor that affects more than one cluster (such as industry-level fixed effects with firm-level clustering). An important exception is when the regressors that are partialed out are cluster fixed effects or fixed effects at a finer level (such as firm-level fixed effects with industry-level clustering), because each of them affects only one cluster.

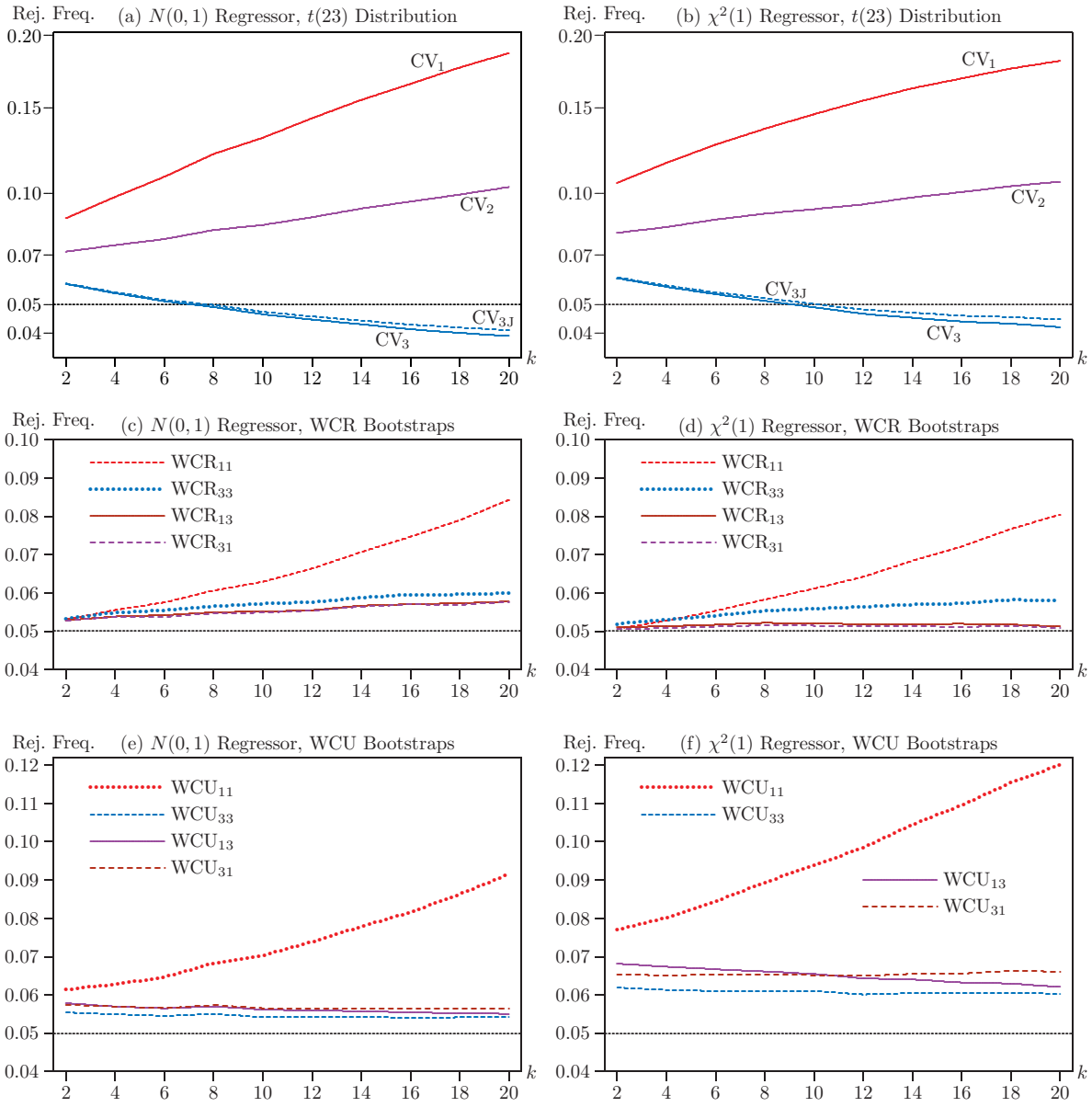
Figure 2 focuses on variation in cluster sizes. In these experiments, there are always 9600 observations, 24 clusters, and 10 regressors. Cluster sizes vary according to (38). Regressors 2 through $k-1$ in (37) are normally distributed according to a random-effects model that yields intra-cluster correlations of 0.50. The test regressor either follows the same normal distribution as the others (in the three panels on the left), or a $\chi^2(1)$ distribution (in the three panels on the right). In the latter case, it is obtained by squaring a normally distributed random variable that is generated by the same random-effects model as the other regressors. The disturbances are also generated by such a model, but with $\rho = 0.10$. We focus on rejection frequencies for a test that $\beta_k = 0$ at the 5% level.

The results for asymptotic tests, based on the $t(23)$ distribution and shown in Panels (a) and (b), are striking. Note that a square-root transformation has been applied to the vertical axis to prevent these panels from being too tall. Tests based on CV_1 over-reject substantially. The extent of the over-rejection increases with γ, and, except for $\gamma = 4$, it is more severe in Panel (b) than in Panel (a). A regressor that follows the $\chi^2(1)$ distribution necessarily has some extreme values, and these become points of high leverage. Not surprisingly, this makes inference more difficult.

Although tests based on CV_2 always reject considerably less often than ones based on CV_1, they also over-reject significantly and to an extent that increases with γ. In contrast, tests based on CV_3 and $\text{CV}_{3\text{J}}$ either under-reject slightly all the time, in Panel (a), or under-reject very slightly for larger values of γ, in Panel (b). The results for CV_3 and $\text{CV}_{3\text{J}}$, which both perform perform remarkably well, are extremely similar. The latter always rejects more often than the former, because the difference between (17) and (18) is the positive semi-definite matrix $((G-1)/G)(\hat{\boldsymbol{\beta}} - \bar{\boldsymbol{\beta}})(\hat{\boldsymbol{\beta}} - \bar{\boldsymbol{\beta}})^\top$. Since CV_3 tends to under-reject slightly in Figure 2, it might seem that $\text{CV}_{3\text{J}}$ is to be preferred. However, as we shall see, there are also many cases in which CV_3 over-rejects, and $\text{CV}_{3\text{J}}$ therefore over-rejects slightly more. Thus, in practice, it would be perfectly reasonable to report either CV_3 or $\text{CV}_{3\text{J}}$. We never encountered a case in which it made any real difference.

The results for the WCR bootstrap tests, shown in Panels (c) and (d), are surprising. In the past, what we are now calling WCR_{11} has been the only variant of the WCR bootstrap, and numerous Monte Carlo experiments have suggested that it is the procedure of choice. But WCR_{33} performs notably better than WCR_{11} for every value of γ, and both WCR_{13} and WCR_{31} perform better still. Remarkably, these two procedures perform almost the same in every case. Oddly, all the WCR procedures perform better in Panel (d), where the test regressor is highly skewed, than they do in Panel (c), where it is Gaussian. At least in part, the rather mediocre performance of WCR_{11} is due to the fact that $k = 10$, which is a larger number than has been used in most previous experiments; see Figure 3 below.

Figure 3: Rejection frequencies as a function of k



Notes: The vertical axes show rejection frequencies for tests of $\beta_k = 0$ in (37) at the .05 level. Results are based on 400,000 replications, with $\gamma = 2$, $\rho = 0.10$, and $B = 399$ bootstrap samples. There are 24 clusters, 9600 observations, and k regressors, where k varies from 2 to 20 by 2.

Some of the results for the WCU bootstrap tests, shown in Panels (e) and (f), are also surprising. It is not a surprise that WCU_{11} rejects more often than WCR_{11} or that its performance is much worse in Panel (f) than in Panel (e). However, the fact that the other three WCU procedures over-reject much less often than WCU_{11} may well be surprising. In both panels, WCU_{33} is clearly the procedure of choice. WCU_{13} and WCU_{31} perform much

better than WCU_{11}, but worse than WCU_{33}. The differences between WCU_{13} and WCU_{31} are small, but larger than the differences between WCR_{13} and WCR_{31} in Panels (c) and (d).

Figure 3 is similar to Figure 2, but the number of regressors k is now on the horizontal axis, and $\gamma = 2$. In Panels (a) and (b), CV_1 over-rejects to an increasing extent as k increases. So does CV_2, although it always over-rejects considerably less than CV_1. In contrast, CV_3 and $\text{CV}_{3\text{J}}$ over-reject modestly for small values of k and under-reject modestly for large ones.

Panels (c) and (d) look a lot like the same panels in Figure 2, even though what is on the horizontal axis is different. WCR_{11} performs quite well for very small values of k, but it over-rejects more and more severely as k increases. WCR_{33} performs much better than WCR_{11}, but WCR_{13} and WCR_{31} perform even better. In Panel (d), where the test regressor is highly skewed, they both perform extremely well for all values of k.

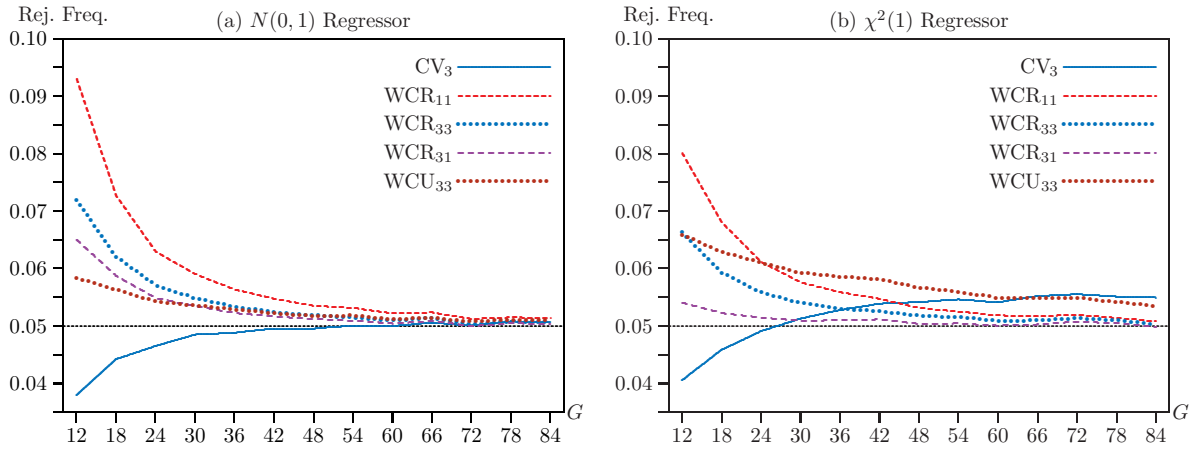
Panels (e) and (f) also look a lot like the same panels in Figure 2. WCU_{11} performs quite poorly, over-rejecting more and more severely as k increases. In contrast, WCU_{33} performs quite well in Panel (e) and fairly well in Panel (f), and there is no tendency for its performance to deteriorate as k increases. As before, the two other bootstrap methods generally perform much better than WCU_{11} but slightly worse than WCU_{33}.

In the next set of experiments, we focus on what happens as G increases. Figure 4 shows rejection frequencies as functions of G, which varies from 12 to 84 by 6, and implicitly also N, since $N = 400G$. In these experiments, $\gamma = 2$ and $k = 10$. In Figures 2 and 3, we reported rejection frequencies for twelve different methods. In Figure 4, however, we reduce this number to five. We omit CV_1 and CV_2, because they never perform very well. Additionally, we omit $\text{CV}_{3\text{J}}$ because it is almost identical to CV_3. Among the restricted bootstrap methods, we report WCR_{11}, because it was until now the procedure of choice. We also report WCR_{33} and WCR_{31}, but we do not report WCR_{13} as it yields results nearly identical to those of WCR_{31}. Among the unrestricted bootstrap methods, we report only WCU_{33}, because it always seems to outperform the other WCU methods.

In Panel (a), using CV_3 with the $t(G-1)$ distribution under-rejects quite noticeably for very small values of G, but it performs extremely well for $G \geq 30$. The bootstrap methods always over-reject, with WCR_{11} always the worst of them. For $G \geq 42$, however, all the bootstrap methods perform very well, with WCR_{31} the winner by a tiny margin.

Panel (b) is more interesting than Panel (a). The extreme skewness of the $\chi^2(1)$ regressor apparently affects the results quite a bit, even when $G = 84$. Although it under-rejects for small values of G, using CV_3 with the $t(G-1)$ distribution over-rejects for larger values, where it is the worst method. We note that $G = 24$ in Figures 2 and 3 is near where the curve for CV_3 crosses the .05 line in Figure 4. The best method is WCR_{31} in every case. It performs remarkably well for $G \geq 30$. However, all three WCR methods perform well for

Figure 4: Rejection frequencies as a function of G



Notes: The vertical axes show rejection frequencies for tests of $\beta_k = 0$ in (37) at the .05 level. Results are based on 400,000 replications, with $\gamma = 2$, $k = 10$, $\rho = 0.10$, and $B = 399$ bootstrap samples. There are between 12 and 84 clusters, all multiples of 6, with 400 observations per cluster on average.

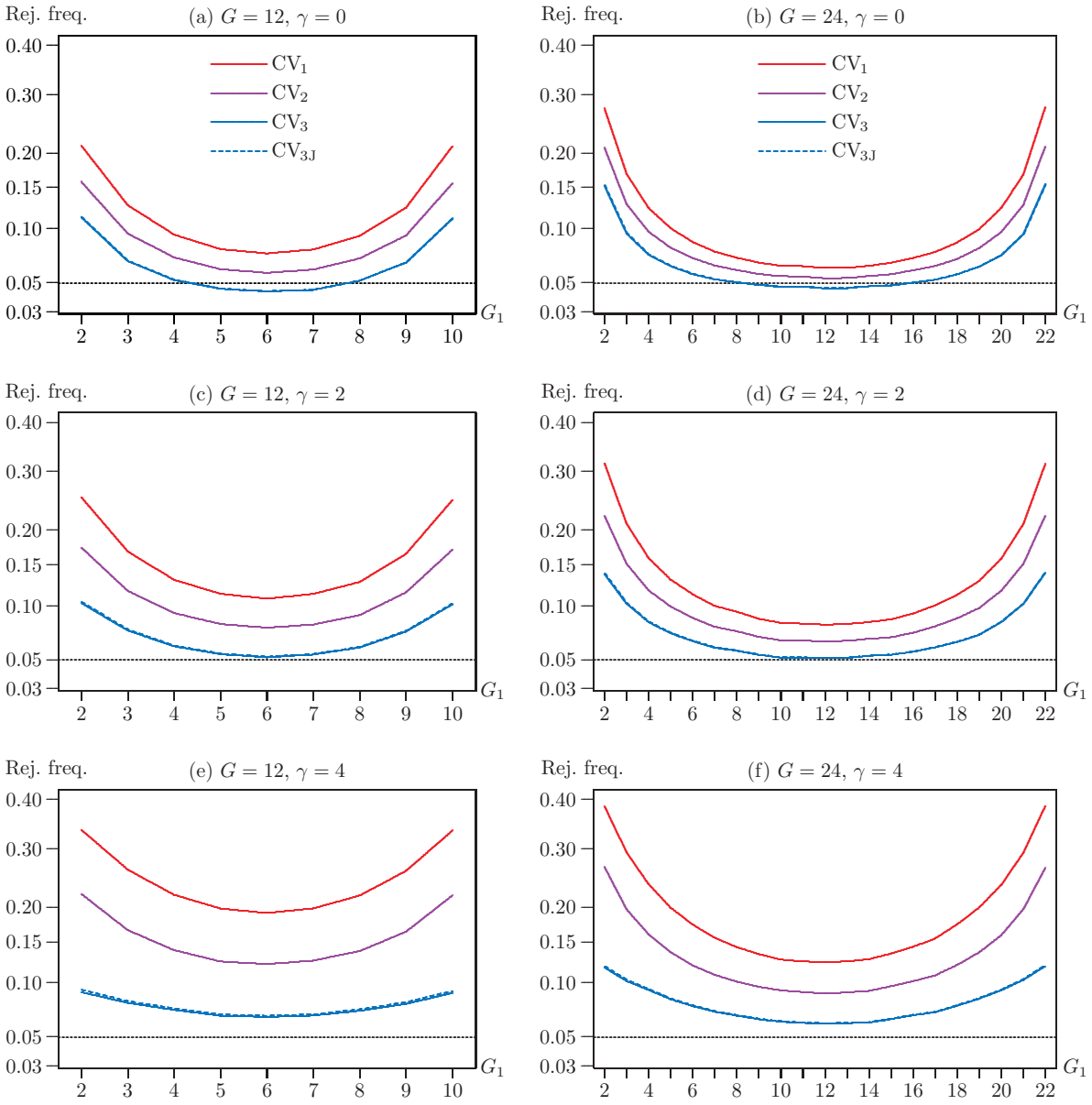
the larger values of G. The only bootstrap method that does not perform particularly well for these values is WCU_{33}. By most standards, of course, every method shown in Panel (b) of Figure 4 works very well, unless G is less than about 30. For $G = 84$, CV_3 is the worst method, but even it rejects only 5.49% of the time. For comparison, CV_1 rejects 9.04% of the time, and CV_2 rejects 7.15%. The best method, WCR_{31}, rejects 4.97% of the time, which is not significantly different from 5%.

Many applications of cluster-robust inference involve treatment at the cluster level, and existing methods generally perform very poorly when either the number of treated clusters or the number of control clusters is small. Using CV_1 with the $t(G-1)$ distribution or WCU_{11} leads to severe over-rejection, and using WCR_{11} leads to severe under-rejection (MacKinnon and Webb 2017, 2018). Our next set of experiments therefore focuses on the model

$$y_{gi} = \beta_1 + \boldsymbol{Z}_{gi}\boldsymbol{\beta}_2 + \beta_k x_g + u_{gi}, \tag{39}$$

where x_g is a treatment dummy, $\boldsymbol{Z}_{gi}$ is a row vector of other regressors, and u_{gi} is generated by a random-effects model with intra-cluster correlation ρ. The treatment dummy equals 1 for G_1 of the G clusters and 0 for the remaining $G_0 = G - G_1$. The clusters that are treated are chosen at random. The $\boldsymbol{Z}_{gi}$ consist of eight more dummy variables. For each of these variables and each cluster, a probability π_g between 0.25 and 0.75 is chosen at random for each replication. Then each observation for that variable in that cluster equals 1 with probability π_g and 0 otherwise. This design is intended to mimic the situation often encountered in treatment regressions, where all of the regressors are dummies. It allows these variables to

Figure 5: Rejection frequencies based on $t(G-1)$ distribution for treatment case



Notes: The vertical axes, which have been subjected to a square-root transformation, show rejection frequencies for tests of $\beta_k = 0$ in (39) at the .05 level. The horizontal axes show G_1, the number of treated clusters. Results are based on 400,000 replications, with $k = 10$ regressors and $\rho = 0.10$. There are either 12 or 24 clusters, with 400 observations per cluster on average. Treated clusters are chosen at random.

vary moderately across clusters.

Figure 5 shows rejection frequencies based on the $t(G-1)$ distribution for six cases. In the left-hand column, there are 12 clusters and 4800 observations. In the right-hand column, there are 24 clusters and 9600 observations. The value of γ is 0 in the top row, 2 in the middle

row, and 4 in the bottom row. The number of treated observations G_1 varies between 2 and $G-2$ on the horizontal axes. It would have been impossible to set $G_1 = 1$ or $G_1 = G-1$, because CV_2, CV_3, and $\text{CV}_{3\text{J}}$ cannot be computed in those cases. For the jackknife-based estimators, this is obvious from (15). When there is just one treated cluster, or just one control cluster, and it happens to be the one that is omitted, then the coefficient of interest in $\hat{\boldsymbol{\beta}}^{(g)}$ is not identified.

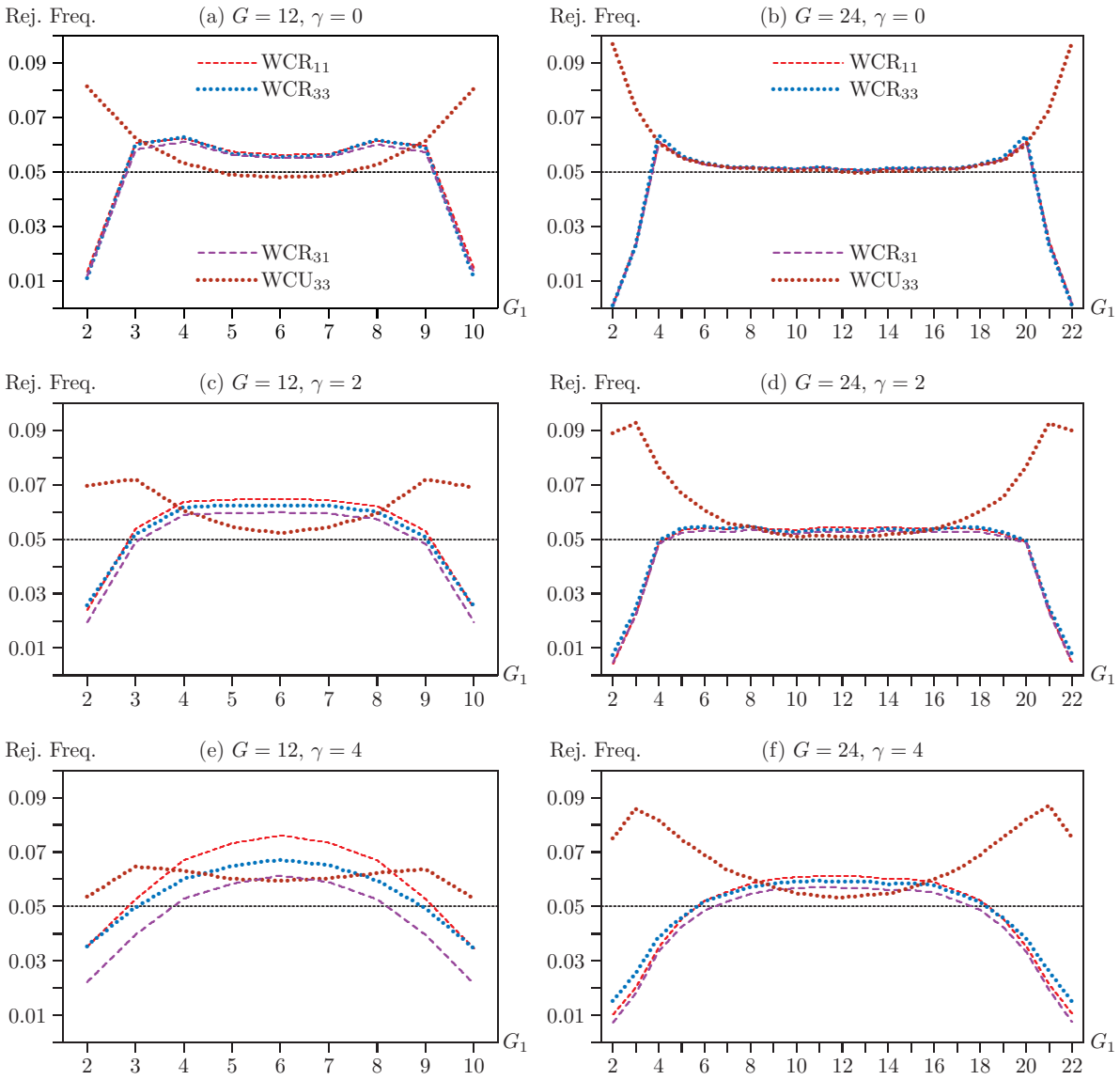
As previous work has shown, tests that use CV_1 tend to over-reject severely when G_1 or $G - G_1$ are small. This is evident in Figure 5. The over-rejection is worst in Panel (f), where both γ and G are largest. CV_2 over-rejects less than CV_1, but it still does not work very well, except perhaps for values of G_1 near $G/2$ when $\gamma = 0$; see Panels (a) and (b). In contrast, CV_3 and $\text{CV}_{3\text{J}}$, which perform almost identically, are much less prone to over-reject than the other two CRVEs. They actually under-reject for values of G_1 fairly near $G/2$ when $\gamma = 0$, and they perform very well for values of G_1 near $G/2$ when $\gamma = 2$. Oddly, CV_3 and $\text{CV}_{3\text{J}}$ over-reject less seriously for extreme values of G_1 when γ is large than when γ is small.

Figure 6 shows results for four bootstrap tests for the same set of experiments as in Figure 5. When $\gamma = 0$, all three variants of the WCR bootstrap perform almost identically. However, as γ increases, their performance starts to differ. WCR_{31} seems to reject least frequently, which is a good thing for intermediate values of G_1 and a bad thing for extreme values. In contrast, WCR_{33} under-rejects least severely for extreme values of G_1. However, for intermediate values, it over-rejects less than WCR_{11} but more than WCR_{31}.

The most surprising results in Figure 6 are the ones for the unrestricted wild bootstraps. We do not report results for WCU_{11} or WCU_{31}, because they would have required a much longer vertical axis. WCU_{11} rejects almost 28% of the time in its worst case ($G = 24$, $G_1 = 2$, $\gamma = 4$), and WCU_{31} rejects over 12% of the time in its worst case ($G = 24$, $G_1 = 2$, $\gamma = 0$). In contrast, WCU_{33} is arguably the best method overall when $G = 12$, and it performs very well for intermediate values of G_1 when $G = 24$. In addition, it never over-rejects as severely as CV_3 for extreme values of G_1.

Although the cluster sizes in our experiments vary greatly when $\gamma = 4$, the largest cluster is not dramatically larger than every other one. Results in Djogbenou et al. (2019) suggest that many methods work poorly when one cluster is much bigger than the others. More than half of all the incorporations in the United States occur in Delaware (Hu and Spamann 2020). This implies that studies of the effects of corporate governance based on changes in state laws, where standard errors are clustered by state of incorporation, are likely to encounter severe errors of inference. To investigate this phenomenon, we create artificial samples with 50 clusters based on data for incorporations by year and state from Spamann and Wilkinson (2019). There are 205,566 observations, of which 108,538, or 52.80%, are for

Figure 6: Bootstrap rejection frequencies for treatment case

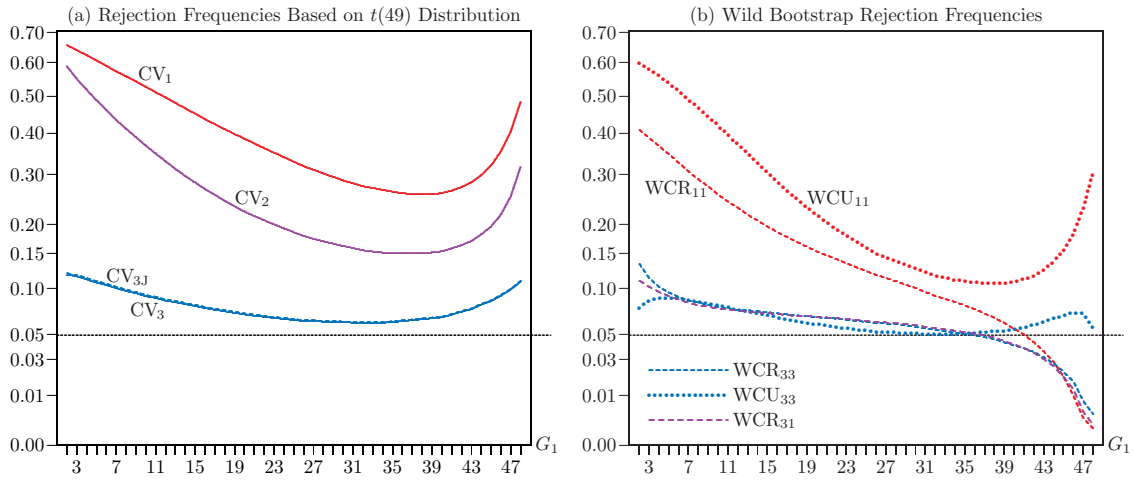


Notes: The vertical axes show rejection frequencies for tests of $\beta_k = 0$ in (39) at the .05 level. The horizontal axes show G_1, the number of treated clusters. Results are based on 400,000 replications, with $k = 10$, $\rho = 0.10$, and $B = 399$ bootstrap samples. There are either 12 or 24 clusters, with 400 observations per cluster on average.

Delaware. The second-largest cluster is Nevada, with 17,010 or 8.27%, and the smallest is Montana, with 101 or 0.05%.

We perform a set of experiments similar to the ones in Figures 5 and 6 using these artificial samples. There are 10 regressors, generated in the same way as before, with one exception. Because investigators are surely aware of whether or not the largest cluster (Delaware) is treated, it is always treated in our experiments. The other clusters to be treated (between

Figure 7: Rejection frequencies when a treated cluster is very large



Notes: The vertical axes show rejection frequencies for tests of $\beta_k = 0$ in (39) at the .05 level. Results are based on 400,000 replications, with $k = 10$, $\rho = 0.10$, and $B = 399$. There are 205,566 observations and 50 clusters, with cluster sizes proportional to incorporations in U.S. states. The largest cluster is always treated, and the other clusters are treated at random. The number of treated clusters varies from 2 to 14 by 1, from 16 to 36 by 2, and then from 38 to 48 by 1.

1 and 47 of them) are chosen at random. Because the largest cluster is always treated, the rejection frequencies are no longer the same for G_1 and $G - G_1$ treated clusters. However, since this is a pure treatment model, the results for G_1 treated clusters that include Delaware must be the same as the results for $G - G_1$ treated clusters that exclude Delaware.

The results in Figure 7 are striking. In Panel (a), using either CV_1 or CV_2 leads to over-rejection that varies between severe and extreme. Using CV_3 and $\text{CV}_{3\text{J}}$ also leads to over-rejection, but it is much less severe. For between 20 and 41 treated clusters, rejection frequencies are less than 0.07. In Panel (b), WCU_{11} over-rejects severely, and WCR_{11} can either over-reject or under-reject, often severely. In contrast, our new bootstrap methods work remarkably well. The best of them is WCU_{33}, which always rejects less than 9% of the time and sometimes rejects just about 5% of the time. WCR_{31} and WCR_{33} also perform much better than WCR_{11}, except when G_1 is very large, in which case they under-reject severely.

Even though it is based on real data, the distribution of cluster sizes in the experiments reported in Figure 7 is very extreme. Although the performance of CV_3 and three of our new bootstrap methods is far from perfect, it is generally very much better than that of existing methods. Thus it appears that jackknife-based methods are remarkably robust to heterogeneity in cluster sizes.

7 Simulations: Test Power

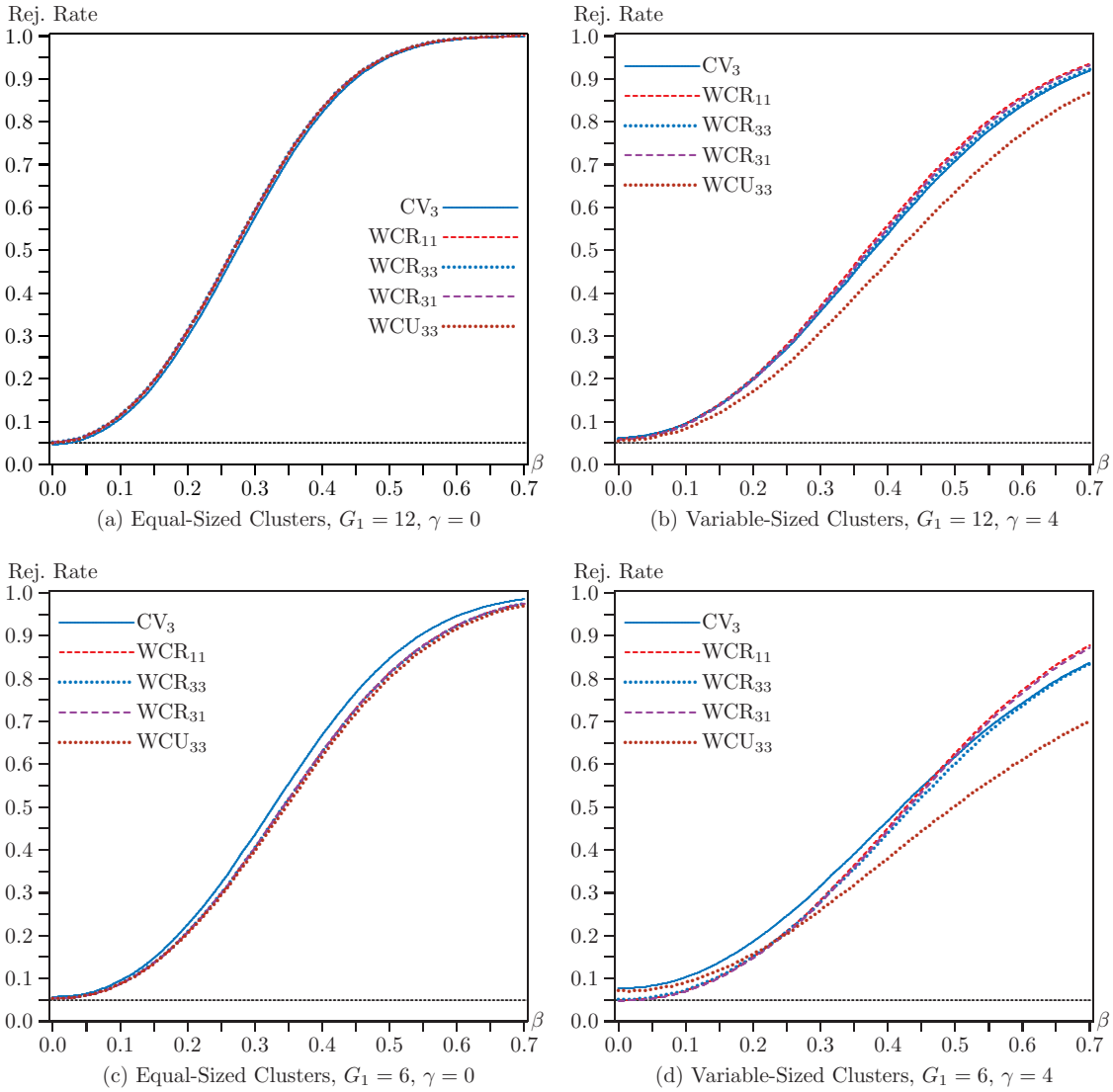
It is natural to worry that a new test may be less powerful than existing tests, especially when it performs much better under the null hypothesis. In this section, we therefore investigate test power. Studying power is tricky, because it is unreasonable to compare tests that have noticeably different rejection frequencies under the null. If, for example, an asymptotic test rejects 15% of the time under the null and a bootstrap test based on it rejects 6% of the time, then we would expect the asymptotic test to have substantially more power than the bootstrap test. But the additional power may be entirely spurious, simply reflecting the finite-sample over-rejection by the asymptotic test.

One way to compare tests with different rejection frequencies under the null is to "size-adjust" them. But this approach has two serious conceptual difficulties. First, size-adjusted tests are infeasible. What do we learn by comparing tests that cannot actually be performed? Second, there are often many ways to size-adjust a given test, and they may yield quite different results. The idea of size-adjustment is to base rejection frequencies for tests under the alternative on critical values calculated by simulation under the null. But, in general, there exists an infinite number of DGPs that satisfy the null hypothesis. If they all yield the same critical values, then there is no problem. But if they yield different critical values, as will often be the case, then we have to choose which null DGP to use. It seems natural to make the null DGP used for critical values as close as possible to the alternative DGP. Davidson and MacKinnon (2006) suggests a particular way of doing this, based on the Kullback-Leibler information criterion, but this approach means using a different critical value for each set of values of the parameters under test.

To avoid the difficulties just discussed, we focus on four cases where the tests of interest all perform quite well under the null. They are treatment experiments similar to the ones in Figures 5 and 6, with $G = 24$, $N = 9600$, and $k = 5$. In Panels (a) and (b), $G_1 = 12$, so that precisely half the clusters are treated. In Panels (c) and (d) $G_1 = 6$, so that the effects of having few treated clusters are apparent but not severe. In order to avoid excessive power loss, we use $B = 999$ for the bootstrap tests. We use $k = 5$ instead of $k = 10$ partly to reduce computational cost and partly to improve test performance under the null.

Figure 8 shows rejection frequencies as a function of β_k, the actual coefficient on the treatment dummy in (39), when the null hypothesis is that $\beta_k = 0$. In Panels (a) and (c), $\gamma = 0$, so that every cluster has exactly 400 observations. In Panel (a), the perfectly balanced case, all five power functions are visually indistinguishable. In Panel (c), where only six clusters are treated, CV_3 has noticeably more power than any of the bootstrap methods, which are all but identical.

Figure 8: Power functions for several tests



(a) Equal-Sized Clusters, $G_1 = 12$, $\gamma = 0$

(b) Variable-Sized Clusters, $G_1 = 12$, $\gamma = 4$

(c) Equal-Sized Clusters, $G_1 = 6$, $\gamma = 0$

(d) Variable-Sized Clusters, $G_1 = 6$, $\gamma = 4$

Notes: The vertical axes show rejection frequencies for tests at the .05 level. Results are based on 400,000 replications, with $G = 24$, $N = 9600$, $k = 5$, $\rho = 0.10$, and $B = 999$. The hypothesis being tested is $\beta_k = 0$ in (39). The horizontal axes show the values of β in the DGP.

In Panels (b) and (d), cluster sizes vary from 32 to 1513. All tests are substantially less powerful than in Panels (a) and (c), because, whenever there is intra-cluster correlation, the information content of a sample declines as the cluster sizes become more variable. The most striking result in both panels is that WCU_{33} has noticeably less power than any of the other methods. This is especially true in Panel (d), where WCU_{33} over-rejects modestly under the null but becomes by far the least powerful method for larger values of β_k. The pattern for CV_3 is similar but much less pronounced. Under the null hypothesis, it over-rejects slightly

under the null in Panel (b) and noticeably in Panel (d), with rejection frequencies of 0.0612 and 0.0775, respectively. But for large enough values of β_k, it has less power than WCR_{11} and WCR_{31}, especially in Panel (d). The latter two methods also have slightly more power than WCR_{33} in Panel (b) and noticeably more in Panel (d) for large values of β_k.

Based on these admittedly limited results, the procedure of choice appears to be WCR_{31}. For larger values of β_k, it is always one of the two most powerful tests. WCR_{11} has similar power, and it also works well under the null in these experiments, but it is much more prone to over-reject than WCR_{31} in Figures 3, 4, 6 and 7.

Cluster-robust standard errors and bootstrap methods are often used to form confidence intervals. Although we do not perform any Monte Carlo experiments explicitly to study the properties of confidence intervals, these can be inferred from Figure 8 and the results in Section 6. Most confidence intervals are implicitly or explicitly obtained by inverting a hypothesis test. When such a test has approximately the correct rejection frequency, the resulting confidence interval must have approximately correct coverage. Similarly, when such a test has high power, the resulting confidence interval must be relatively short.

In many of the experiments in Section 6, tests based on CV_3 and the $t(G-1)$ distribution are much less prone to over-reject than tests based on CV_1. This suggests that the coverage of confidence intervals based on CV_3 standard errors will often be much better than the coverage of ones based on CV_1 standard errors. Even more reliable intervals may often (but not always) be obtained by using the WCR_{31} or WCR_{33} bootstraps, which perform much better than the well-known WCR_{11} bootstrap in many cases. The WCU_{33} bootstrap also performs well in many cases under the null, but the results in Panels (b) and (d) of Figure 8 suggest that, when cluster sizes vary a lot, intervals based on it may be longer than ones based on WCR_{33}, which in turn may be slightly longer than ones based on WCR_{31}.

Based on its excellent performance in many of the experiments of Section 6 and the fact that it seems to have slightly better power than WCR_{33} in Panels (b) and (d) of Figure 8, we tentatively recommend that confidence intervals should be obtained by inverting WCR_{31} bootstrap tests. However, inverting WCR_{33} bootstrap tests, or simply using CV_3 standard errors and the $t(G-1)$ distribution, would often lead to very similar intervals. It is probably a good idea to use more than one method in practice.

Of course, it is easier to obtain a confidence interval by using a standard error and the $t(G-1)$ distribution than by inverting a bootstrap test, and it is easier to invert any form of WCU bootstrap test than any form of WCR bootstrap test. However, the computational cost of inverting WCR bootstrap tests can be remarkably small, even for very large samples; see Roodman et al. (2019, Section 3.5) and MacKinnon (2022, Section 3.4).

8 Empirical Example

In this section, we consider an empirical example based on MacKinnon et al. (2022a, Section 8). It exploits differences in the minimum wage across states and years to estimate the impact of minimum wages on hours worked for teenagers.

Data at the individual level from the American Community Survey (ACS) are obtained from IPUMS (Ruggles et al. 2020) and cover the years 2005–2019. The minimum wage data come from Neumark (2019) and are collapsed to state-year averages to match the ACS frequency. We restrict attention to teenagers aged 16–19, keeping only individuals who are children of the respondent to the survey and who have never been married. We drop individuals who had completed one year of college by age 16 and those reporting in excess of 60 hours usually worked per week. We also restrict attention to individuals who identify as either black or white. There are 492,827 observations in 51 clusters, which correspond to all 50 states plus the District of Columbia.

The model we estimate is

$$y_{ist} = \alpha + \beta \mathrm{mw}_{st} + \boldsymbol{Z}_{ist}\boldsymbol{\gamma} + \mathrm{year}_t\,\boldsymbol{\delta}_t + \mathrm{state}_s\,\boldsymbol{\delta}_s + u_{ist}, \tag{40}$$

where y_{ist} is usual hours worked per week for individual i. The parameter of interest is β, which is the coefficient on mw_{st}, the minimum wage in state s at time t. The row vector $\boldsymbol{Z}_{ist}$ collects a large set of individual-level controls, including race, gender, age, and education. There are also year and state fixed effects.

As MacKinnon et al. (2022a) discusses, clustering could in principle be done at several different levels, but the one that is most appealing and seems to be supported by the data is clustering at the state level. This is therefore the only level that we use. The 51 clusters vary considerably in size. The smallest has 258 observations, and the largest has 35,995. The ratio of these numbers is more than twice as large as for $\gamma = 4$ in the experiments of Section 6. The mean number of observations per cluster is 9,663, and the median is 7,082. This suggests that inference based on CV_1 and the $t(50)$ distribution may not be reliable. Other measures of cluster heterogeneity, which are discussed in the original paper, lead to the same conclusion.

Table 1 presents our key results. As expected, the CV_3 t-statistic is somewhat smaller than the CV_1 t-statistic, and the P value based on the $t(50)$ distribution is therefore somewhat larger. The four WCR P values are larger than either of them, but still below 0.05, and they are remarkably similar to each other. The four WCU P values are notably smaller than the WCR ones, and again they are very similar to each other. However, because we used a very large number of bootstrap replications, $B = 999,999$, we are confident that WCR_{31} and WCR_{33} actually do yield larger P values than WCR_{11} and WCR_{13}.

Table 1: Hours and Minimum Wage Example

	Estimate	Std. error	t-statistic	P value
CV_1	−0.15389	0.06231	−2.4697	0.0170
CV_3	−0.15389	0.06713	−2.2925	0.0261
	Wild cluster bootstrap P values			
WCR_{11}	0.0362	WCU_{11}	0.0207	
WCR_{13}	0.0352	WCU_{13}	0.0186	
WCR_{31}	0.0374	WCU_{31}	0.0227	
WCR_{33}	0.0371	WCU_{33}	0.0203	

Notes: There are 492,827 observations and 51 clusters. Bootstrap P values use $B = 999,999$. All the numbers in this table were obtained in 2 minutes and 14 seconds using one core of an Intel i9-10850K processor running at 3.6 GHz.

Based on how similar the four WCR P values are, and on how well many of the WCR methods perform in the experiments of Section 6, we tentatively conclude that the P value for the test of $\beta = 0$ is probably between 0.034 and 0.039. Thus the null hypothesis can safely be rejected at the .05 level but not at the .01 level.

9 Concluding Remarks

Until recently, the only CRVE for linear regression models that was computationally feasible for samples with large clusters was the one usually called CV_1. Since it often leads to serious over-rejection and under-coverage, it was widely recommended to use the original version of the wild cluster restricted bootstrap proposed by Cameron et al. (2008) instead. This is the version that we now call the WCR_{11} bootstrap. In Section 3, however, we have shown how to compute another CRVE, usually known as CV_3 (Bell and McCaffrey 2002), in a computationally efficient fashion by using the fact that it is a cluster jackknife estimator. As shown in Section 6, inference based on CV_3, even without bootstrapping, seems to be much more reliable than inference based on CV_1, and sometimes even more reliable than inference based on the widely-used WCR_{11} bootstrap.

In Section 5, we prove some simple, but by no means obvious, algebraic results about the relationship between cluster jackknife estimates and score vectors at the cluster level. These allow us to obtain several new variants of the wild cluster bootstrap, all of which are easy to compute. Based on the simulation results in Section 6, three of them seem to be particularly interesting. These are the methods we call WCR_{31}, WCR_{33}, and WCU_{33}. In all cases, the first subscript identifies the bootstrap DGP, and the second subscript identifies the variance

matrix estimator. Thus, for example, WCR_{31} uses restricted bootstrap scores that have been modified by using the jackknife transformation given in (34), along with the usual CV_1 standard errors. In contrast, WCU_{33} uses unrestricted bootstrap scores modified using the jackknife transformation (31), along with CV_3 standard errors. Perhaps surprisingly, WCU_{33} often performs as well as or better than the two new WCR bootstrap methods under the null, but it seems to be less powerful than they are when cluster sizes are unbalanced; see Section 7.

Two of the new restricted wild bootstrap methods, WCR_{31} and WCR_{33}, tend to yield very similar results and often seem to be more reliable than WCR_{11}. However, when they do differ noticeably, WCR_{31} tends to be the winner, both under the null and under the alternative. We therefore recommend, somewhat tentatively, that WCR_{31} should always be employed. Of course, unless it yields definitive results, it would be wise to try a few other methods as well. The obvious choices are CV_3 with $t(G-1)$, WCR_{11}, WCR_{33}, and WCU_{33}.

In an empirical example with 51 clusters that vary greatly in size, all four WCR bootstraps yield extremely similar results, which are more conservative than ones based on either CV_1 or CV_3 and the $t(50)$ distribution. They are also more conservative than ones based on any of the WCU bootstraps. Of course, we would expect to see greater variability in the results of alternative methods when the clusters are fewer in number and/or more heterogeneous.

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