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# MEMORANDUM

## No 21/2014

# Practical Correlation Bias Correction in Two-way Fixed Effects Linear Regression



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## Practical correlation bias correction in two-way fixed effects linear regression

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#### Abstract

When doing two-way fixed effects OLS estimations, both the variances and covariance of the fixed effects are biased. A formula for a bias correction is known, but in large datasets it involves inverses of impractically large matrices. We detail how to compute the bias correction in this case.

*Keywords:* Limited mobility bias, Two way fixed effects, Linear regression *JEL*: C13, C33, C55, C87

#### 1. Introduction

We consider a model of the type:

$$y = X\beta + D\theta + F\psi + \epsilon, \tag{1}$$

where  $y \in \mathbb{R}^n$  is an outcome, X is a matrix of covariates, D is an  $n \times k_{\theta}$  matrix resulting from dummy encoding a factor, F is an  $n \times k_{\psi}$  matrix resulting from dummy encoding another factor, and  $\epsilon$  is a normally distributed error term. This is a perfectly ordinary least squares system, but our assumption is that  $k_{\theta}$  and  $k_{\psi}$  are large, e.g. of the order  $10^5-10^7$ . This creates some computational challenges. The canonical example in the panel data econometrics literature of this kind of model can be found in [1], where the outcome y is the wage, D is a matrix of dummies for each individual, and F is a matrix of dummies for each firm.  $\theta$  are time-constant individual fixed effects,  $\psi$  are time-constant firm fixed effects. They study the correlation  $cor(D\theta, F\psi)$  as a way to investigate whether "high wage" workers tend to work in "high wage" firms.

We assume that  $\beta$ ,  $\theta$ ,  $\psi$ , and  $\epsilon$  are estimated by OLS, e.g. with the methods in [7, 10, 17, 19]. It is shown in [3] that the variances  $\tilde{\sigma}_{\theta}^2 = \operatorname{var}(D\hat{\theta})$  and  $\tilde{\sigma}_{\psi}^2 = \operatorname{var}(F\hat{\psi})$  are positively biased, and that the covariance  $\tilde{\sigma}_{\theta\psi} = \operatorname{cov}(D\hat{\theta}, F\hat{\psi})$  is typically negatively biased, and they give explicit formulas for the magnitude of the biases. The biases can be substantial, and can even change the sign of the correlation estimate:  $\tilde{\rho}_{\theta\psi} = \frac{\tilde{\sigma}_{\theta\psi}}{\sqrt{\tilde{\sigma}_{\theta}^2 \tilde{\sigma}_{\psi}^2}}$ . This particular type of bias is known as *limited mobility* bias.

A challenge with the bias correction formulas in [3] is that they involve the inverses of large square matrices, of size  $k_{\theta}$  and  $k_{\psi}$ . Given that these quantities can be of the order  $10^5-10^7$ , the method is impractical to use directly with commonly available computing contraptions. Some authors acknowledge the possible bias, but do not compute it, e.g. [6, 8, 9, 12, 20]. We therefore venture to evaluate the bias correction expressions in [3] without handling any large matrices. Our contributions are mainly in section 5, but for completeness and consistency of notation we include a derivation of the bias expressions from [3] in sections 3 and 4.

In applications there can be other sources of bias than the one corrected by the methods presented here. To solve such bias problem, other models should be used, as in [5, 16]. It is also pointed out in the literature, e.g. in [6], that the OLS assumption of independently identically distributed errors is dubious in some applications, though the bias expressions and the methods in section 5 can probably be adapted to at least some other error structures.

#### 2. Preliminaries

We fix some notation and recall some standard facts about (orthogonal) projections. In general, we let I denote the identity matrix of appropriate size. We assume tacitly that our matrices are of the appropriate size. For a matrix A we denote by R(A) its column space, or range. We denote by  $M_A$ the projection onto the orthogonal complement of R(A). Note that in general,  $M_A = M_A^t = M_A^2$  by the defining property of projections. For A of full column rank, we have

$$M_A = I - A(A^t A)^{-1} A^t, (2)$$

but  $M_A$  is defined for any matrix A. For two matrices A and B we denote by  $M_{A,B} = M_{B,A}$  the intersection  $M_A \wedge M_B$ , the projection onto the complement of the column space of the block matrix  $\begin{bmatrix} A & B \end{bmatrix}$ . In general,  $M_{A,B}M_A = M_AM_{A,B} = M_{A,B}$ , and  $M_{A,B}A = 0$ . A standard result in operator theory is that if  $\mathbf{R}(A)$  is orthogonal to  $\mathbf{R}(B)$ , or if  $\mathbf{R}(A) \subset \mathbf{R}(B)$ , then  $M_{A,B} = M_AM_B = M_BM_A$ . We denote by  $\mathbf{1} = (1, 1, \ldots, 1)$  a vector of the appropriate length where each coordinate equals 1. Thus,  $M_{\mathbf{1}}$  is the projection which subtracts the mean.

We will now and then use the defining property of the trace, tr(AB) = tr(BA), without mentioning. With this notation, we may state some assumptions for our system in (1). There is no intercept in X. We have removed a reference group from  $\psi/F$ . There are no more collinearities in the system; in the language of [2], there is a single *connected group*, or *connected component*. These assumptions are necessary for identification of  $\hat{\theta}$  and  $\hat{\psi}$ . In particular,  $M_{F,X}D$  and  $M_{D,X}F$  are assumed to be of full column rank, so that both  $D^t M_{F,X}D$  and  $F^t M_{D,X}F$  are invertible. We also have  $M_D M_1 = M_1 M_D = M_D$ . We do not assume that X is small, i.e. X may, among other covariates, contain one or more high dimensional dummy encoded factors, as in [7].

This lemma will come in handy later:

Lemma 2.1. If A and B are matrices, then  $M_{A,B} = M_A M_{M_AB}$ . If  $M_A B$  has full column rank, we have  $M_{A,B} = M_A - M_A B (B^t M_A B)^{-1} B^t M_A$ .

*Proof.* First, note that  $M_A(I - M_{A,B})$  is a projection. Let  $P = I - M_{M_AB}$ . P is the projection onto the range of  $M_AB$ , i.e.  $\mathbb{R}(P) = \mathbb{R}(M_AB)$ . We show that  $\mathbb{R}(M_AB) = \mathbb{R}(M_A(I - M_{A,B}))$ . Note that  $\mathbb{R}(M_AB)$  is spanned by the columns of  $M_AB$ , i.e.  $\mathbb{R}(M_AB) = M_A \mathbb{R}(B)$ . On the right hand side the columns of  $I - M_{A,B}$  span  $\mathbb{R}(A) + \mathbb{R}(B)$ . So that  $\mathbb{R}(M_A(I - M_{A,B})) = M_A(\mathbb{R}(A) + \mathbb{R}(B)) = M_A \mathbb{R}(B)$ . Two projections with the same range are equal, so  $P = M_A(I - M_{A,B}) = M_A - M_{A,B}$ . Substituting P, we obtain  $I - M_{M_AB} = M_A - M_{A,B}$ . Multiplying through with  $M_A$  yields  $M_A - M_A M_{M_AB} = M_A - M_{A,B}$ , which can be rewritten as  $M_{A,B} = M_A M_{M_AB}$ . In the case that  $M_AB$  has full column rank, we have from (2) that  $M_{M_AB} = I - M_A (B^{t} M_A B)^{-1} B^t M_A$ . □

Remark 2.2. Given a vector v we note that [10, Algorithm 3.1] gives a procedure by which we can compute  $M_{D,F}v$ . It is not mentioned explicitly in [10] that the same method can be used to compute  $M_Av$  for an arbitrary  $n \times k$  matrix A, not only for matrices arising from dummy-encoding. The theory and algorithm is the same, but the actual computation of each projection in [10, Algorithm 3.1(2) and (15)] corresponding to columns of A, is slightly more complicated. Such a procedure has been implemented in [11] through implementation of interactions between factors and continuous covariates; one may use a factor with a single level. In the present paper, there is also no intrinsic dependence on D and F being dummy encoded factors, most of the theory (except we don't need a reference group, and  $M_1M_D \neq M_D$ ) is the same if D and F are interactions between factors and covariates, or something else; but the author knows of no such application.

#### 3. Variances and covariance bias

When deriving the bias correction formulas, we will follow the exposition in [3], but change the notation to reflect our emphasis on the projections of the type  $M_A$ , which we can compute.

As in [3, (8–10)], we have a biased sample estimate for the variance of  $D\theta$ :

$$\tilde{\sigma}_{\theta}^2 = \frac{\hat{\theta}^t D^t M_1 D\hat{\theta}}{n},\tag{3}$$

for the variance of  $F\psi$ :

$$\tilde{\sigma}_{\psi}^2 = \frac{\hat{\psi}^t F^t M_1 F \hat{\psi}}{n},\tag{4}$$

and for the covariance:

$$\tilde{\sigma}_{\theta\psi} = \frac{\hat{\theta}^t D^t M_1 F \hat{\psi}}{n}.$$
(5)

We take the expectation as in [3, (16)]:

$$\mathbb{E}(\tilde{\sigma}_{\theta}^2) = \mathbb{E}\left(\frac{\hat{\theta}^t D^t M_1 D\hat{\theta}}{n}\right) = \frac{\theta^t D^t M_1 D\theta}{n} + \frac{\operatorname{tr}(D^t M_1 D \operatorname{Var}(\hat{\theta}))}{n}$$
(6)

using the general formula for the expectation of a quadratic form

$$\mathbb{E}(x^{t}Ax) = \mathbb{E}(x^{t})A\mathbb{E}(x) + \operatorname{tr}(A\operatorname{Var}(x))$$
(7)

with  $A = D^t M_1 D$  and  $x = \hat{\theta}$ .

We are interested in the term  $\sigma_{\theta}^2 = (\theta^t D^t M_1 D \theta)/n$ . We can readily estimate the left hand side of (6) as  $\tilde{\sigma}_{\theta}^2$  from the OLS estimate  $\hat{\theta}$ . To find the bias, i.e. the trace term in (6), we need an expression for  $\operatorname{Var}(\hat{\theta})$ . The problem is the same for  $\tilde{\sigma}_{\psi}^2$  and  $\tilde{\sigma}_{\theta\psi}$ , but we detail it only for the  $\theta$  case.

Remark 3.1. We note that the bias problem is symmetric in  $\theta$  and  $\psi$ , even though not all our formulas will be syntactically symmetric. Also,  $\tilde{\sigma}^2_{\theta}$ ,  $\tilde{\sigma}^2_{\psi}$ , and  $\tilde{\sigma}_{\theta\psi}$  do not depend on which reference group we have picked, neither do they depend on whether the reference group is in  $\theta$  or  $\psi$ . Indeed,  $M_1 D\hat{\theta}$  and  $M_1 F \hat{\psi}$  are independent of where the reference group is. To see this, a change of reference group has the same effect on  $D\hat{\theta}$  and  $F\hat{\psi}$  as a transformation of the type  $D\hat{\theta} \mapsto D\hat{\theta} - \alpha \mathbf{1}$ ,  $F\hat{\psi} \mapsto F\hat{\psi} + \alpha \mathbf{1}$ . But we have  $M_1 \mathbf{1} = 0$ . That is, in e.g. (6), both  $\tilde{\sigma}^2_{\theta}$  and  $\sigma^2_{\theta}$  are independent of the whereabouts of the reference group, so the trace term is independent of it as well. For simplicity, we do assume that the reference group is in  $\psi$ .

We may find a formula for  $Var(\hat{\theta})$  via the Frisch-Waugh-Lovell theorem. By multiplying through (1) with  $M_{F,X}$  we have

$$M_{F,X}y = M_{F,X}D\theta + M_{F,X}\epsilon.$$

By standard OLS assumptions we have

$$\hat{\theta} = \theta + (D^t M_{F,X} D)^{-1} D^t M_{F,X} \epsilon,$$

and, by using the i.i.d. assumption  $\operatorname{Var}(\epsilon) = \sigma_{\epsilon}^2 I$ , we obtain

$$\operatorname{Var}(\hat{\theta}) = (D^t M_{F,X} D)^{-1} D^t M_{F,X} \operatorname{Var}(\epsilon) M_{F,X} D (D^t M_{F,X} D)^{-1}$$
$$= \sigma_{\epsilon}^2 (D^t M_{F,X} D)^{-1}.$$
(8)

As usual,  $\sigma_{\epsilon}^2$  can be estimated from the residuals  $\hat{\epsilon}$  when solving (1) by OLS.

That is, the bias term for  $\tilde{\sigma}_{\theta}^2$  in (6) is

$$\delta_{\theta} = \hat{\sigma}_{\epsilon}^2 \operatorname{tr}((D^t M_{F,X} D)^{-1} D^t M_1 D)/n.$$
(9)

It is the  $k_{\theta} \times k_{\theta}$  matrix inside the trace term which may be too large to be handled directly, as in [3, p. 687].

We may rewrite

$$\operatorname{tr}((D^{t}M_{F,X}D)^{-1}D^{t}M_{1}D) = \operatorname{tr}(M_{1}D(D^{t}M_{F,X}D)^{-1}D^{t}M_{1}) = \operatorname{tr}(Q^{t}Q) \ge 0,$$

with  $Q = (D^t M_{F,X} D)^{-1/2} D^t M_1$ , so the bias is non-negative. By symmetry between  $\theta$  and  $\psi$ , the corresponding bias term for  $\tilde{\sigma}_{\psi}^2$  is:

$$\delta_{\psi} = \hat{\sigma}_{\epsilon}^2 \operatorname{tr}((F^t M_{D,X} F)^{-1} F^t M_1 F)/n.$$
(10)

For the covariance in (5), note the general algebraic formula for a quadratic form with  $A = A^{t}$ , sometimes referred to as a polarization identity:

$$(x+y)^t A(x+y) = x^t A x + 2x^t A y + y^t A y.$$

That is,

$$x^{t}Ay = \frac{1}{2} \left( (x+y)^{t}A(x+y) - x^{t}Ax - y^{t}Ay \right).$$

We use this and (7) on (5), with  $x = D\hat{\theta}$ ,  $y = F\hat{\psi}$ , and  $A = M_1$ . An algebraic excursion yields:

$$\mathbb{E}(\tilde{\sigma}_{\theta\psi}) = \frac{1}{n} (\theta^t D^t M_1 F \psi + \sigma_{\epsilon}^2 \operatorname{tr}(M_1 D (D^t M_{F,X} D)^{-1} D^t M_{F,X} M_{D,X} F (F^t M_{D,X} F)^{-1} F^t)).$$

As in [3], we can use Lemma 2.1 to write:  $M_{D,X} = M_X (I - D(D^t M_X D)^{-1} D^t M_X)$ . We obtain  $D^t M_{F,X} M_{D,X} F = -D^t M_{F,X} D (D^t M_X D)^{-1} D^t M_X F$  and rewrite the trace term as:

$$-\operatorname{tr}(M_{1}D(D^{t}M_{X}D)^{-1}D^{t}M_{X}F(F^{t}M_{D,X}F)^{-1}F^{t}),$$

or, as in [3, (22)]

$$\delta_{\theta\psi} = -\sigma_{\epsilon}^2 \operatorname{tr}(D^t M_1 F (F^t M_{D,X} F)^{-1} F^t M_X D (D^t M_X D)^{-1})/n.$$
(11)

*Remark* 3.2. We see from the formulas that the magnitude of the bias increases with  $\sigma_{\epsilon}^2$ , ceteris paribus. Although unobserved heterogeneity does not bias the OLS estimates, it does bias non-linear functions of them, such as  $\tilde{\sigma}_{\theta}^2$ . Other error structures than  $\operatorname{Var}(\epsilon) = \sigma_{\epsilon}^2 I$  can be accomodated by changing equation (8), provided an estimate for  $Var(\epsilon)$  can be found.

#### 4. Independent covariates

In the special case when we have no X, or the columns of X are orthogonal to both D and F, we may simplify the bias correction formulas (9), (10), and (11) by observing that since R(X) is orthogonal to R(D) and R(F), we have  $M_X D = D$ , and  $M_X F = F$ . Also,  $M_{D,X} = M_D M_X$ , so that  $M_{D,X} F =$  $M_D M_X F = M_D F$ , similarly  $M_{F,X} D = M_F D$ . From (2) we also have  $D(D^t D)^{-1} D^t = I - M_D$ .

We then obtain:

$$\begin{aligned} \delta'_{\theta} &= \hat{\sigma}_{\epsilon}^{2} \operatorname{tr}((D^{t}M_{F}D)^{-1}D^{t}M_{\mathbf{1}}D)/n, \\ \delta'_{\psi} &= \hat{\sigma}_{\epsilon}^{2} \operatorname{tr}((F^{t}M_{D}F)^{-1}F^{t}M_{\mathbf{1}}F)/n, \\ \delta'_{\theta\psi} &= -\hat{\sigma}_{\epsilon}^{2} \operatorname{tr}((F^{t}M_{D}F)^{-1}F^{t}(I-M_{D})M_{\mathbf{1}}F)/n. \end{aligned}$$

Using  $(I - M_D)M_1 = M_1 - M_D$ , and  $(M_1 - M_D)^2 = M_1 - M_D$ , we note that

$$\begin{aligned} \delta'_{\theta\psi} &= -\hat{\sigma}_{\epsilon}^2 \operatorname{tr}((M_1 - M_D)F(F^t M_D F)^{-1}F^t(M_1 - M_D))/n \\ &= -\hat{\sigma}_{\epsilon}^2 \operatorname{tr}(Q^t Q) \leq 0, \end{aligned}$$

with  $Q = (F^t M_D F)^{-1/2} F^t (M_1 - M_D)$ . We may also rewrite:

$$\begin{aligned} \delta_{\theta\psi}' &= \hat{\sigma}_{\epsilon}^2 \operatorname{tr}((F^t M_D F)^{-1} F^t (M_D - M_1) F)/n \\ &= \hat{\sigma}_{\epsilon}^2 \operatorname{tr}((F^t M_D F)^{-1} F^t M_D F)/n - \hat{\sigma}_{\epsilon}^2 \operatorname{tr}((F^t M_D F)^{-1} F^t M_1 F)/n \\ &= \hat{\sigma}_{\epsilon}^2 \operatorname{tr}(I)/n - \delta_{\psi}' \\ &= \hat{\sigma}_{\epsilon}^2 \frac{k_{\psi}}{n} - \delta_{\psi}'. \end{aligned}$$

In particular, we have  $\delta'_{\psi} \ge \sigma_{\epsilon}^2 \frac{k_{\psi}}{n}$ . By Remark 3.1, we also have

$$\delta_{\theta\psi}' = \hat{\sigma}_{\epsilon}^2 \frac{k_{\theta} - 1}{n} - \delta_{\theta}',$$

where we replace  $k_{\psi}$  with  $k_{\theta} - 1$  in the numerator because of the reference group. This means we can write  $\delta'_{\psi}$  in terms of  $\delta'_{\theta}$ :

$$\delta'_{\psi} = \delta'_{\theta} - \hat{\sigma}_{\epsilon}^2 \frac{k_{\theta} - 1 - k_{\psi}}{n}.$$

That is, when the covariates X are uncorrelated with the factors D and F, the bias corrections are:

$$\begin{split} \delta'_{\theta} &= \hat{\sigma}_{\epsilon}^{2} \operatorname{tr}((D^{t} M_{F} D)^{-1} D^{t} M_{1} D)/n &\geq \hat{\sigma}_{\epsilon}^{2} \frac{k_{\theta} - 1}{n}, \\ \delta'_{\psi} &= \delta'_{\theta} - \hat{\sigma}_{\epsilon}^{2} \frac{k_{\theta} - 1 - k_{\psi}}{n} &\geq \hat{\sigma}_{\epsilon}^{2} \frac{k_{\psi}}{n}, \\ \delta'_{\theta\psi} &= -\delta'_{\theta} + \hat{\sigma}_{\epsilon}^{2} \frac{k_{\theta} - 1}{n} &\leq 0. \end{split}$$

This is a computational advantage, since it suffices to compute a single trace.

#### 5. Computing the trace

Computing the trace of a matrix is simple in theory, it is just to sum the diagonal elements. However, if the matrices in (9), (10), and (11) are too large to be handled by commonly available computers, we need some other method. Luckily, quantum physicists and others have studied such problems for quite some time. The following is one approach.

By using (7) with an x with  $\mathbb{E}(x) = 0$  and  $\operatorname{Var}(x) = I$ , we obtain

$$\operatorname{tr}(A) = \mathbb{E}(x^t A x).$$

The right hand side can be estimated by sample means. It is shown in [13] that if we limit ourselves to real vectors, i.e.  $x \in \mathbb{R}^m$ , the least variance in  $x^t A x$  with symmetric A is obtained by drawing x as sign vectors, i.e. uniformly in  $\{-1, 1\}^m$ . This method is also described in [4, Proposition 4.1].

That is, to compute the bias term  $\delta_{\theta}$  in (9), we estimate the expectation in:

$$\delta_{\theta} = \hat{\sigma}_{\epsilon}^2 \mathbb{E}(x^t M_1 D (D^t M_{F,X} D)^{-1} D^t M_1 x) / n, \tag{12}$$

by sample means. This entails drawing an  $x \in \{-1, 1\}^n$ , then solve the equation

$$D^t M_{F,X} Dv = D^t M_1 x, (13)$$

for v by e.g. a conjugate gradient method (CG) like the one in [15, Algorithm 3], and compute  $x^t M_1 Dv$ . This will be repeated a number of times and then averaged. The CG method has the advantage that it does not require a matrix representation of the linear operator  $D^t M_{F,X} D$ , it is sufficient with a procedure for computing the matrix-vector product, like the one in Remark 2.2. The same method is used to compute the other bias-terms. We then obtain unbiased estimates for the variances and covariances, and may estimate the correlation.

The bias term for  $\tilde{\sigma}_{\psi}^2$  is obtained from the bias term for  $\tilde{\sigma}_{\theta}^2$  by interchanging F and D in (12):

$$\delta_{\psi} = \hat{\sigma}_{\epsilon}^2 \mathbb{E}(x^t M_1 F (F^t M_{D,X} F)^{-1} F^t M_1 x) / n.$$
(14)

The bias term for  $\tilde{\sigma}_{\theta\psi}$  becomes, from (11):

$$\delta_{\theta\psi} = -\hat{\sigma}_{\epsilon}^2 \mathbb{E}(x^t M_1 F (F^t M_{D,X} F)^{-1} F^t M_X D (D^t M_X D)^{-1} D^t M_1 x) / n.$$
(15)

Each sample requires two steps. We draw an  $x \in \{-1, 1\}^n$ , and solve

$$D^t M_X Dv = D^t M_1 x,$$

for v. Then we solve

$$F^t M_{D,X} F w = F^t M_X D v,$$

for w. Finally, we compute  $x^t M_1 F w$ .

Remark 5.1. The operators  $M_D$ ,  $M_F$ ,  $M_{F,X}$ ,  $M_{D,X}$ , and  $M_X$  are applied repeatedly in the CG iterations described above. The operators  $M_D$  and  $M_F$  are just centering on the means, i.e. subtraction of the group means. In general, by Remark 2.2, given a vector  $\lambda$ ,  $M_X\lambda$ ,  $M_{F,X}\lambda$ , and  $M_{D,X}\lambda$  can be computed by the methods in [10], but unless X contains high dimensional dummy encoded factors, it is wise to use Lemma 2.1 to write  $M_{F,X} = M_F M_{M_FX}$ , and  $M_{D,X} = M_D M_{M_DX}$ , i.e. to apply two simpler operators in succession. We can precompute  $M_F X$  and  $M_D X$ , and orthonormalize the columns; if the columns  $a_i$  of A are orthonormal, then  $M_A \lambda$  is easy to compute:  $M_A \lambda = \lambda - \sum_i \langle \lambda, a_i \rangle a_i$ , where  $\langle \cdot, \cdot \rangle$ is the Euclidean inner product. That is, applying  $M_{F,X}$ ,  $M_{D,X}$  and  $M_X$  do not involve the possibly costly iterations of [10]. After orthonormalization we may anyway use that algorithm; with orthogonal columns it will terminate after one iteration. A fast, though numerically unstable, algorithm for orthonormalizing the columns of A, yielding a matrix Y with the same range as A, is  $Y = A(L^t)^{-1}$ where L is the Cholesky decomposition of  $A^{t}A = LL^{t}$ . We clearly have R(A) = R(Y), and it is readily seen that the columns of Y are orthonormal:  $Y^tY = L^{-1}A^tA(L^t)^{-1} = L^{-1}LL^t(L^t)^{-1} = I$ . If  $A^tA$  is close to singular a more stable algorithm should be used. However, this happens only if  $M_D X$ ,  $M_F X$ or X are close to being column rank deficient, which means that our original system in (1) is close to collinear. Respecifying the model is then probably a better option.

#### 6. Summary

Given the model (1), and OLS estimates  $\hat{\theta}$ ,  $\hat{\psi}$ , and  $\hat{\sigma}_{\epsilon}^2$ . To compute an estimate  $\hat{\rho}_{\theta\psi}$  for  $\rho_{\theta\psi} = \operatorname{cor}(D\theta, F\psi)$ , we compute the biased estimates  $\tilde{\sigma}_{\theta}^2$ ,  $\tilde{\sigma}_{\psi}^2$ , and  $\tilde{\sigma}_{\theta\psi}$  as in eqs. (3), (4), and (5). We then estimate bias correction terms (12), (14), and (15) with sample means as in Section 5, with uniformly drawn  $x \in \{-1, 1\}^n$ :

$$\delta_{\theta} = \hat{\sigma}_{\epsilon}^{2} \mathbb{E}(x^{t} M_{\mathbf{1}} D (D^{t} M_{F,X} D)^{-1} D^{t} M_{\mathbf{1}} x)/n,$$

$$\delta_{\psi} = \hat{\sigma}_{\epsilon}^{2} \mathbb{E}(x^{t} M_{\mathbf{1}} F (F^{t} M_{D,X} F)^{-1} F^{t} M_{\mathbf{1}} x)/n,$$

$$\delta_{\theta\psi} = -\hat{\sigma}_{\epsilon}^{2} \mathbb{E}(x^{t} M_{\mathbf{1}} F (F^{t} M_{D,X} F)^{-1} F^{t} M_{X} D (D^{t} M_{X} D)^{-1} D^{t} M_{\mathbf{1}} x)/n.$$
(16)

The unbiased variances and covariance are:

$$\hat{\sigma}^2_{ heta} = \tilde{\sigma}^2_{ heta} - \delta_{ heta}$$
 $\hat{\sigma}^2_{\psi} = \tilde{\sigma}^2_{\psi} - \delta_{\psi}$ 
 $\hat{\sigma}_{ heta\psi} = \tilde{\sigma}_{ heta\psi} - \delta_{ heta\psi}$ 

We then estimate the correlation  $\rho_{\theta\psi} = \operatorname{cor}(D\theta, F\psi)$  between  $D\theta$  and  $F\psi$  as

$$\hat{\rho}_{\theta\psi} = \frac{\hat{\sigma}_{\theta\psi}}{\sqrt{\hat{\sigma}_{\theta}^2 \hat{\sigma}_{\psi}^2}}.$$

If there are no covariates X, or they are uncorrelated with D and F, the bias corrections in (16) can be replaced with the ones from Section 4:

$$\begin{split} \delta'_{\theta} &= \hat{\sigma}_{\epsilon}^2 \, \mathbb{E}(x^t M_{\mathbf{1}} D (D^t M_F D)^{-1} D^t M_{\mathbf{1}} x)/n, \\ \delta'_{\psi} &= \delta'_{\theta} - \hat{\sigma}_{\epsilon}^2 \frac{k_{\theta} - 1 - k_{\psi}}{n}, \\ \delta'_{\theta\psi} &= -\delta'_{\theta} + \hat{\sigma}_{\epsilon}^2 \frac{k_{\theta} - 1}{n}. \end{split}$$

Alternatively, the symmetric equations can be used:

$$\begin{split} \delta'_{\psi} &= \hat{\sigma}_{\epsilon}^2 \, \mathbb{E}(x^t M_{\mathbf{1}} F (F^t M_D F)^{-1} F^t M_{\mathbf{1}} x) / n, \\ \delta'_{\theta} &= \delta'_{\psi} - \hat{\sigma}_{\epsilon}^2 \frac{k_{\psi} + 1 - k_{\theta}}{n}, \\ \delta'_{\theta\psi} &= -\delta'_{\psi} + \hat{\sigma}_{\epsilon}^2 \frac{k_{\psi}}{n}. \end{split}$$

Remark 6.1. In some cases  $k_{\theta}$  or  $k_{\psi}$  are small enough that matrices of such size can be handled, as in [3, Section 5]. In that case  $\delta'_{\theta}$  or  $\delta'_{\psi}$  can be computed directly, e.g. with

$$\delta'_{\psi} = \hat{\sigma}_{\epsilon}^2 \operatorname{tr}((F^t M_D F)^{-1} F^t M_1 F)/n_{\epsilon}$$

and we avoid sampling to estimate the trace.

#### 7. Implementation suggestions

Application of the large matrices D,  $D^t$ , F, and  $F^t$  is simple in the software system R([18]). These sparse matrices are represented as *factors*, and are applied by subsetting for D and F, and by the function 'rowsum()' for their transposes. Similar mechanisms for handling sparse matrices are often available in other software systems. Efficient application of the matrix operators  $M_D$ ,  $M_F$ ,  $M_{F,X}$ ,  $M_{D,X}$  and  $M_X$  is described in Remark 5.1. Also, note that, due to the way we have formulated the computations in section 5, it is actually not necessary to remove a reference group from the factors at all. The CG-algorithm will converge to one of many possible solutions as in [14], but the ambiguity is annihilated by subsequent computations.

The CG method for solving an equation Ax = b can easily be used for multiple vectors at the same time, i.e. with b a matrix of column vectors. The implementation in [11] of the computation  $M_A v$  can also use a v which is a matrix, parallelizing over the columns of v, thus speeding up the computation. That is, when sampling the expectations in (12), (14), and (15), we can draw multiple vectors and use a matrix x of column vectors.

Since the expectations used to compute the bias corrections are estimated by sample means, they can be computed to arbitrary precision by taking enough samples. We can monitor the sample standard deviation and stop sampling when a desired relative accuracy in  $\hat{\sigma}_{\theta}^2$  and  $\hat{\sigma}_{\psi}^2$  has been reached. If we estimate  $\hat{\sigma}_{\theta}^2$  and  $\hat{\sigma}_{\psi}^2$  first, we can stop sampling for  $\delta_{\theta\psi}$  when a desired absolute accuracy in  $\hat{\rho}_{\theta\psi}$  has been reached. Also, the termination criterion for the CG algorithm can be set to finish when a solution just good enough for our expectation tolerance has been found. A suitable termination criterion can be found in [15]. However, computing a too imprecise solution can introduce bias, and also increase the variance in the expectation sampling, so that more samples may be needed.

Preliminary trials with  $n = 3 \cdot 10^6$ ,  $k_{\theta} = 3 \cdot 10^5$ ,  $k_{\psi} = 3 \cdot 10^4$ , bias and CG precision at 0.01, a true correlation of 0.3, and a biased correlation of 0.15, reveal that typically the required number of samples for the expectations are  $\leq 10$ , which is 1–3 iterations on a 4-cpu computer, decreasing in n. The time requirements are 2–5 m. However, the number of required samples depends on  $\hat{\sigma}_{\epsilon}^2$ , the reason is that the larger  $\hat{\sigma}_{\epsilon}^2$  is, the more accurately we have to estimate the traces to achieve the same precision in  $\hat{\sigma}_{\theta}^2$ ,  $\hat{\sigma}_{\psi}^2$ , and  $\hat{\sigma}_{\theta\psi}$ . Fortunately, in practice there is typically not much heterogeneity left in (1) after controlling for  $\beta$ ,  $\theta$  and  $\psi$ , i.e. the more covariates in X, the smaller  $\sigma_{\epsilon}^2$ . With large n, a case could be made for using only a single sample, this is what we do when we estimate  $\theta = \mathbb{E}(\hat{\theta})$  with the "single sample"  $\hat{\theta}$ . By using 4 samples, relaxing the CG-tolerance so we only do 6 CG-iterations, and assuming the covariates X are independent of D and F, we obtain a correlation within 0.02 of the correct one in about 30 s.

A trial with a real dataset without covariates X, and a biased correlation of  $\approx -0.18$ , with  $k_{\theta} = 2.3 \times 10^6$ ,  $k_{\psi} = 62000$  and  $n = 18 \times 10^6$  takes  $\approx 35$  m. With relaxed precision it finishes in 4 m, with the corrected correlation differing by 0.03 from the 0.01-precision estimate.

We should however keep in mind that our unbiased estimates  $\hat{\sigma}_{\theta}^2$ ,  $\hat{\sigma}_{\psi}^2$ , and  $\hat{\sigma}_{\theta\psi}$  still may be incorrect due to ordinary regression errors in the estimates  $\hat{\theta}$ ,  $\hat{\psi}$ , and  $\hat{\sigma}_{\epsilon}^2$ .

An implementation of these bias corrections will be made available in a future version of [11].

#### 8. References

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