HOW LFE WORKS

SIMEN GAURE

Abstract. Here is a proof for the demeaning method used in lfe, and a description of the methods used for solving the residual equations. As well as a toy-example. This is a preliminary version of [3]. This method, formulated as the Gauss-Seidel algorithm, was noted in [4] without the author noticing it in the first version of this paper.

1. Introduction

We assume we have an OLS model in matrix form

\[ Y = X\beta + D\alpha + \epsilon \]

where \( X \) is a \((n \times k)\)-matrix, and \( D \) is a \((n \times g)\)-matrix. \( D \) is a set of dummies for \( e \) category variables. I.e. \( D \) is a block matrix, \( D = [D_1 \ D_2 \ \cdots \ D_e] \). That is, the entries of each \( D_i \) consists of 0 and 1, with only one non-zero entry per row. These are the dummies from a single factor, one column per level. Hence, the columns of each \( D_i \) are pairwise orthogonal. Though, in general, \( D_i \) is not orthogonal to \( D_j \) for \( i \neq j \).

That is, in R the model will be

\[ Y \sim X_1 + X_2 + \ldots + X_k + D_1 + D_2 + \ldots + D_e \]

where \( D_1, D_2, \ldots, D_e \) are arbitrary factors. I.e. an entirely ordinary model which may easily be estimated by \texttt{lm}, or with sparse-versions of the same.

\( g \) is the sum of the number of levels in the factors. Now, suppose \( g \approx 10^6 \), indeed, assume that all the factors have many levels, so that an unmanageable number of dummies will be created when we try to estimate, even if we sweep out the largest with a within transformation.

Then, we must do the math. Let’s write the model in a slightly different block matrix form, to get hold of some facts of the Frisch-Waugh-Lovell theorem:

\[ Y = \begin{bmatrix} X & D \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} + \epsilon \]

We get the normal equations

\[ \begin{bmatrix} X & D \end{bmatrix}' \begin{bmatrix} X & D \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \begin{bmatrix} X & D \end{bmatrix}' Y \]

which, when multiplied out, become

\[ \begin{bmatrix} X'X & X'D \\ D'X & D'D \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \begin{bmatrix} X'Y \\ D'Y \end{bmatrix} \]

We then write them as two rows

\[ \begin{bmatrix} X'Y \\ D'Y \end{bmatrix} \]

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and assume, for a moment, that we have removed sufficient reference levels from \( D \), so that \( D' D \) is invertible. Now, multiply through equation (3) with \( X' D (D' D)^{-1} \) and subtract equation (2) from (3). This removes the \( \alpha \)-term from (3). We then name \( P = I - D (D' D)^{-1} D' \) to get
\[
X' P \hat{X} = X' Y.
\]

Now, note that \( P \) is a projection, i.e. \( P = P' = P^2 \), hence we have \( X' P X = X' P' P X = (P X)' P X \) and \( X' P Y = X' P' P Y = (P X)' P Y \) which yields
\[
(P X)' P \hat{X} = (P X)' P Y
\]
which is the normal equation of the system
\[
PY = PX \hat{X} + P \epsilon.
\]

That is, \( \hat{X} \) may be estimated from system (5), with the dummies removed, taking into account the adjusted degrees of freedom when computing the covariance matrix.

Moreover, by multiplying through equation (3) with \( D (D' D)^{-1} \) and noting that \( D (D' D)^{-1} D' = I - P \), we get
\[
(I - P) X \hat{X} + D \hat{\alpha} = (I - P) Y
\]
which may be reordered as
\[
Y - (X \hat{X} + D \hat{\alpha}) = PY - PX \hat{X}
\]
showing that the residuals of the projected system (5) equals the residuals of the original system (1). Similarly, the \( \hat{X} \) part of the covariance matrix of (1) can be shown to be identical to the covariance matrix of (5).

All this is well-known as the Frisch-Waugh-Lovell theorem, and is not the main point here, that’s why we’re still in the “Introduction”-section.

2. What \texttt{lfe} does about this

The problem is to compute the projection \( P \), so that we may estimate \( \hat{X} \) from (5). Whenever \( e = 1 \), i.e. a single factor, applying \( P \) amounts to subtracting the group-means. This is known as the within-groups transformation, or centering on the means, or demeaning. But, what does it look like when we have more factors?

Here’s the idea behind \texttt{lfe}, from [3]:

For each of the factors, we have a demeaning projection \( P_i = I - D_i (D_i' D_i)^{-1} D_i' \). This is the projection onto the orthogonal complement of the range (column space) of \( D_i \), called \( R(D_i)^\perp \). These are easy to compute, it’s just to subtract the means of each level. Similarly, \( P \) is the projection on \( R(D)^\perp \). This one is not yet obvious how to compute.

There is a relation between all these range-spaces:
\[
R(D)^\perp = R(D_1)^\perp \cap R(D_2)^\perp \cap \cdots \cap R(D_e)^\perp.
\]
To see this, consider a vector \( v \in R(D)^\perp \). By definition, it’s orthogonal to every column in \( D \), hence to every column in every \( D_i \), thus \( v \) is in the intersection on
the right hand side. Conversely, take a $v$ which is in all the spaces $R(D_i)$. It’s orthogonal to every column of every $D_i$, hence it’s orthogonal to every column in $D$, so it’s in $R(D)$. This relation may be written in terms of projections:

$$P = P_1 \land P_2 \land \cdots \land P_e.$$ 

Now, there’s a theorem about projections [5, Theorem 1] stating that for every vector $v$, we have

$$Pv = \lim_{n \to \infty} (P_1 P_2 \cdots P_e)^n v. \quad (7)$$

So, there’s how to compute $Pv$ for an arbitrary vector $v$, just demean it with each projection in succession, over and over, until it gives up. We do this for every column of $X$ and $Y$ to find $PY$ and $PX$, and then we may solve $\hat{\beta}$ from (4). This procedure has been wrapped up with a threaded C-routine in the function `felm`. Thus, the $X_1, X_2, \ldots, X_k$ can be estimated efficiently by

```
fe(lm(Y ~ X1 + X2 + \ldots + Xk | D1 + D2 + \ldots + De))
```

If there is only one factor (i.e. $e = 1$), this reduces to the within-groups model.

3. THE DUMMIES?

To find $\hat{\alpha}$, the coefficients of all the dummies, we may write (6) as

$$D\hat{\alpha} = (Y - X\hat{\beta}) - (PY - PX\hat{\beta})$$

where the right hand side is readily computed when we have completed the steps above. There will be no more than $e$ non-zeros in each row of $D$. This type of sparse system lends itself to solving by the Kaczmarz method ([6]).

The Kaczmarz method may be viewed as a variant of (7), specifically for solving linear equations. (Though, historically, the Kaczmarz-method predates Halperin’s more general Hilbert-space theorem by 25 years.) The idea is that in a matrix equation like

$$Dx = b$$

we may view each row of the system $(d_i, x) = b_i$ as an equation defining a hyperplane $Q_i$ (where $d_i$ is the $i$'th row of $D$). The solution set of the system is the intersection of all the hyperplanes $Q = Q_1 \cap Q_2 \cap \cdots \cap Q_n$. Thus, again, if the projection onto each $Q_i$ is easy to compute (it is $x \mapsto x + (b_i - \langle d_i, x \rangle) d_i/\|d_i\|^2$), we may essentially use (7) on these projections to find a vector in the intersection, starting from the zero-vector.

In our case, each row $d_i$ of the matrix $D$ has exactly $e$ non-zero entries, which are all equal to unity. This makes the computation of the projection on each $Q_i$ easy and fast. We don’t have to care about rank-deficiency (you do, if you’re going to interpret the results); but we do remove consecutive duplicate rows, as these are just repeated applications of the same projection, and thus contribute nothing to the result (because projections by definition are idempotent.)

Anyway, the Kaczmarz method converges to a solution $\hat{\alpha}$. Since we use 0 as our starting point, we compute the projection of the zero-vector onto the solution space, this is, by a defining property of projections, the solution with minimal norm. We must then apply some estimable function to get interpretable coefficients, the package supplies a couple to choose from. Moreover, it’s easy to get different
solutions by using different vectors as starting points. Estimable functions should evaluate to the same value for any two such solutions, this is utilized to test user-supplied functions for estimability in the function \texttt{is.estimable}.

From the Kaczmarz method we don’t get any indication of the rank-deficiency. Though for \( e = 2 \), this can be inferred from the component-structure returned by \texttt{getfe}. The method requires little memory, and it’s way faster than most other methods.

A drawback is that the Kaczmarz method is not immediately parallelizable (though there’s a variant by Cimmino which is, each iteration projects the point onto each hyperplane, then the next approximation is the centroid of these projections), and it does not yield any covariance matrix or standard errors. However, it is fast, so it’s possible to bootstrap the standard errors if that’s desired.

A benchmark real dataset used during development contained 15 covariates, approx 20,000,000 observations, with 2,300,000 levels in one of the factors, and 270,000 in the other. Centering the covariates takes approx 2 hours (on 8 CPUs), and then computing the fixed effects by the Kaczmarz-method takes about 4 minutes (on 1 CPU). Bootstrapping the standard errors (112 times) takes about 14 hours. (It is not necessary to centre the covariates over again when bootstrapping, only the resampled residuals. These are generally faster to centre than arbitrary covariates.) This is the default method used by \texttt{getfe}.

Alternatively, one may choose a sparse Cholesky solver. That is, we have from (3) that

\[
D'D\hat{\alpha} = D'(Y - X\hat{\beta}).
\]

In the case \( e = 1 \), we have that \( D'D \) is diagonal, this is the within-groups case, and \( \hat{\alpha} \) is just the group-means of the residuals \( Y - X\hat{\beta} \). In the general case, we have a large, but sparse, linear system. This may be solved with the methods in package \texttt{Matrix}. This procedure has been packaged in the function \texttt{getfe}.

Now, it turns out that identification, hence interpretation, of the coefficients, may be a complicated affair. The reason is that the matrix \( D'D \) may be rank-deficient in unexpected ways. It’s sometimes not sufficient to remove a reference-level in each factor. In the case \( e = 2 \) these difficulties are well understood and treated in [1] and [2], as well as implemented in \texttt{lfe}. For larger \( e \), this problem is harder, \texttt{lfe} uses a pivoted Cholesky-method to find linear dependencies in \( D'D \), and removes them, but the resulting interpretation of the coefficients are in general not well understood. (This, of course, applies to the Kaczmarz method as well).

4. Interactions

The above discussion about the method, indeed the discussion in [3], does not use anywhere that the matrix \( D \) contains only zeros and ones, except in the concrete computation of projections. If we interact one or more factors with some continuous covariates, the entire theory goes through unchanged. The centring is slightly different, involving covariates; likewise the Kaczmarz step. Beginning with version 1.6, \texttt{lfe} supports projecting out such interactions, e.g.

\[
Y \sim X1 + X2 \mid X3:D1 + D2 + D3
\]

The estimability analysis discards interaction terms, i.e. it assumes that all coefficients for \( X3:D1 \) are identified. Note that the terms in the second part of
5. Optimization potential

Profiling with the tool “perf” on linux, reveals that there is some potential for optimizations in both the centering process and the Kaczmarz-solver. Both suffer from memory-bandwidth limitations, leading to an “Instructions Per Cycle”-count in some cases below 0.3 (where the theoretical maximum is 2 or 4), despite being almost pure floating point operations. This depends heavily on the problem size, cache architecture of the CPU, number of cores in use, memory bandwidth and latency, and the CPU-speed. I haven’t figured out a good solution for this, though I haven’t given it a lot of thought.

An interesting optimization would be to use a GPU for these operations. They are quite simple, and thus quite well suited for coding in OpenCL, CUDA or similar GPU-tools, and could possibly yield an order of magnitude speedup, though I haven’t tried anything of the sort.

6. An example

First we create a couple of covariates:

```r
set.seed(41)
x <- rnorm(500)
x2 <- rnorm(length(x))
x3 <- rnorm(length(x))
```

Then we create some random factors, not too many levels, just for illustration, and some effects:

```r
f1 <- factor(sample(7,length(x),replace=TRUE))
f2 <- factor(sample(4,length(x),replace=TRUE))
f3 <- factor(sample(3,length(x),replace=TRUE))
eff1 <- rnorm(nlevels(f1))
eff2 <- rexp(nlevels(f2))
eff3 <- runif(nlevels(f3))
```

Then we create an outcome with some normal residuals:

```r
y <- x + 0.5*x2 + 0.25*x3 + eff1[f1] + eff2[f2] + eff3[f3] + rnorm(length(x))
```

Now, for illustration, create a demeaning function according to (7):

```r
demean <- function(v,f1) {
Pv <- v; oldv <- v-1
while(sqrt(sum((Pv-oldv)**2)) >= 1e-7) {
  oldv <- Pv
  for(f in f1) Pv <- Pv - ave(Pv,f)
}
Pv
}
```

and demean things
fl <- list(f1,f2,f3)
Py <- demean(y,fl)
Px <- demean(x,fl)
Px2 <- demean(x2,fl)
Px3 <- demean(x3,fl)

And then we estimate it

summary(lm(Py ~ Px + Px2 + Px3 - 1))
##
## Call:
## lm(formula = Py ~ Px + Px2 + Px3 - 1)
##
## Residuals:
## Min 1Q Median 3Q Max
## -2.7367 -0.6249 -0.0114 0.7014 3.0506
##
## Coefficients:
## Estimate Std. Error t value Pr(>|t|)
## Px 1.06543 0.04484 23.761 < 2e-16 ***
## Px2 0.50988 0.04541 11.228 < 2e-16 ***
## Px3 0.22739 0.04346 5.232 2.48e-07 ***
## ---
## Signif. codes: 0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
##
## Residual standard error: 0.991 on 497 degrees of freedom
## Multiple R-squared: 0.586, Adjusted R-squared: 0.5835
## F-statistic: 234.5 on 3 and 497 DF, p-value: < 2.2e-16

Note that \texttt{lm} believes there are too many degrees of freedom, so the standard errors are too small.

The function \texttt{felm} in package \texttt{lfe} adjusts for the degrees of freedom, so that we get the same standard errors as if we had included all the dummies:

\begin{verbatim}
library(lfe, quietly=TRUE)
summary(est <- felm(y ~ x + x2 + x3 | f1+f2+f3))
##
## Call:
## felm(formula = y ~ x + x2 + x3 | f1 + f2 + f3)
##
## Residuals:
## Min 1Q Median 3Q Max
## -2.7367 -0.6249 -0.0114 0.7014 3.0506
##
## Coefficients:
## Estimate Std. Error t value Pr(>|t|)
## x 1.06543 0.04539 23.472 < 2e-16 ***
## x2 0.50988 0.04597 11.092 < 2e-16 ***
## x3 0.22739 0.04346 5.168 3.46e-07 ***
\end{verbatim}
We also illustrate how to fetch the group coefficients. Since there are no identification problems in this dataset, we use an estimable function identical to the one in \texttt{lm} when using treatment contrasts. (Though, a similar function is available with \texttt{ef='ref'} which is the default for \texttt{getfe}).

```r
def <- function(v,addnames) {
    r1 <- v[[1]]
    r2 <- v[[8]]
    r3 <- v[[12]]
    result <- c(r1+r2+r3,v[2:7]-r1,v[9:11]-r2,v[13:14]-r3)
    if(addnames) names(result) <- c(1,'(Intercept)',
        paste('f1',2:7,sep='.',pa),
        paste('f2',2:4,sep='.',pa),
        paste('f3',2:3,sep='.'))
    result
}
# verify that it's estimable
is.estimable(def,est$fe)
```

Get the same estimation in \texttt{lm}, with dummies:

```r
summary(lm(y ~ x + x2 + x3 + f1 + f2 + f3))
```

# Call:
## lm(formula = y ~ x + x2 + x3 + f1 + f2 + f3)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -2.7367 -0.6249  0.0114  0.7014  3.0506
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.76603    0.15590   24.16 < 2e-16 ***
## x            1.06543    0.04539   23.47 < 2e-16 ***
## x2           0.50988    0.04597   11.09 < 2e-16 ***
## x3           0.22739    0.04400    5.17  3.46e-07 ***
## f12          -1.66030    0.17676   -9.39 < 2e-16 ***
## f13          -4.55768    0.17337  -26.29 < 2e-16 ***
## f14           0.13910    0.17691    0.79   0.4321
## f15          -3.76258    0.16676  -22.56 < 2e-16 ***
## f16          -1.13283    0.16892  -6.71  5.57e-11 ***
## f17          -1.30707    0.17473  -7.48  3.50e-13 ***
## f22           1.27199    0.12711  10.01  < 2e-16 ***
## f23           0.17046    0.12771    1.34   0.1826
## f24           2.08417    0.12497  16.68  < 2e-16 ***
## f32          -0.15765    0.11320  -1.39   0.1633
## f33           0.22157    0.11314  -1.96   0.0508 .
##
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 1
##
## Residual standard error: 1.003 on 485 degrees of freedom
## Multiple R-squared:  0.8425, Adjusted R-squared:  0.8379
## F-statistic: 185.3 on 14 and 485 DF,  p-value: < 2.2e-16

**References**


*Ragnar Frisch Centre for Economic Research, Oslo, Norway*