Fitting linear, generalized linear and mixed models to large data sets

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Conclusions
Are my data a “large” data set?

- Computing hardware and software evolves rapidly (my DVD player runs \texttt{R}). We must apply an evolving standard for what constitutes a “large” data set.

- Your data are not large if using the naive (i.e. the “blunt instrument” or \texttt{fortune(122)}) approach takes less time than finding and reading the documentation that describes how to do what you want to do efficiently.

- If you find that the naive approach runs out of memory or takes a long time you can
  - Send an email message to R-help with a subject like “R is SOOOOOO SLOOOOOOW” and vaguely describe what you are trying to do and why this software is so bad. (Do keep an asbestos suit handy for the \texttt{fortune(9)} response.)
  - Try the \texttt{fortune(138)} approach.
What is the effect of large data?

- In short, you need to think about the computation and how it is to be done.
- Early texts on statistical computing (Chambers, 1975 or Kennedy and Gentle, 1980) emphasized algorithms for numerical linear algebra, simulation, optimization, etc. paying careful attention to the time and space requirements.
- In modern environments we don’t bother with “counting flops” because we realize that setting up the numerical computation often dominates the time spent actually doing the computation (fortune(98)).
- Large data sets can change that balance. All that hard earned knowledge of how the cost of various operations changes with the size of the matrices involved
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Models and model matrices

- One of the underappreciated aspects of the S language is the ability to combine a formula and a data set to produce model frame and a model matrix. It is not as trivial as it may seem.
- Most operations with an \( n \times p \) model matrix \( X \) and a response vector \( y \) are some form of least squares (e.g. iteratively reweighted least squares).
- Everything you learned in a linear algebra class doesn’t apply to computational linear algebra. (“No, Virginia, least squares computations are not really done as \((X'X)^{-1}X'y\).”)
- Numerical analysts recognize two direct decomposition methods (QR and Cholesky) for linear least squares. The time complexity is \( np^2 \) for both. Space complexity is \( p^2 \) for Cholesky and \( np \) for QR. (The “sweep” operator used by SAS is not even considered a contender.)
The sweep-based method used by SAS is used because it can detect and remove rank deficiencies (in a way different from how numerical analysts would do it).

The problem of rank deficiencies occurs less frequently in the S language implementation but still frequently enough that it must be taken into consideration. This is why the QR decomposition in R is still based on Linpack, not Lapack.

Standard numerical linear algebra software doesn’t quite do things the way that statisticians want to (and numerical analysts don’t seem to want to make the necessary changes).
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Cholesky versus QR

- The Cholesky method can be row-oriented (i.e. it can operate on horizontal sections of $X$ and $y$).
- The QR method is column-oriented.
- In theory, $R$ provides the option of using Cholesky or QR (there is a method argument to `lm.fit`). In practice it only allows QR. (See previous discussion of rank deficiency.) “In theory, theory and practice are the same. In practice, they’re not.”
- QR has somewhat better numerical properties than Cholesky. If this matters your $X$ is close to rank deficient.
What can you do with existing dense matrix software?

• You could work on horizontal sections of $X$ and $y$ (biglm package) with a Cholesky decomposition.

• If you use iterative reweighting then you must store all of $X$ somewhere or regenerate it from the model frame and the formula at each iteration.
Is $n$ large, $p$ moderate, or are $n$ and $p$ both large?

- If $p$ is getting large as $n$ gets large, what causes $p$ to get large?
- Do you have “nuisance parameters” associated with experimental (observational) units? If so, they should probably be modeled as random effects.
- If the linear predictor involves nuisance parameters, that part of the model matrix will end up being sparse.
- If you model the effects of units as fixed effects you need to watch for rank deficiencies. When modeled as random effects the “shrinkage” behavior of the BLUPs provides the regularization.
- For this type of data and model the combination of mixed-effects models and sparse matrix techniques is highly effective.
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An example

'data.frame': 1721024 obs. of  9 variables:
$ instr  : Factor w/ 7964 levels "10000","10001",..: 1 1 1 1 1 1 1 1 1 1 ...
$ dept   : Factor w/ 106 levels "AERO","AFAM",..: 43 43 43 43 43 43 43 43 43 43 ...
$ id     : Factor w/ 54711 levels "9000000001","9000000002",..: 12152 1405 ...
$ nclass : num  40 29 33 13 47 49 37 14 21 20 ...
$ vgpa   : num  NA NA NA NA NA NA NA NA NA NA ...
$ rawai  : num  2.88 -1.15 -0.08 -1.94 3.00 ...
$ gr.pt  : num  4 1.7 2 0 3.7 1.7 2 4 2 2.7 ...
$ section: Factor w/ 70366 levels "19959 AERO0011A001",..: 18417 18417 ...
$ semester: num  19989 19989 19989 19989 19989 19972 ...
An initial model fit

```r
> system.time(m1 <- lmer(gr.pt ~ (1|id) + (1|instr) + (1|dept),
                     anon.grades.df, verbose = 1))
```

```
0: 3661278.9: 0.294219 0.111907 0.0127038
1: 3449897.0: 0.759218 0.360591 0.862370
2: 3447850.7: 0.933685 0.418499 0.797016
3: 3447432.7: 0.872045 0.462103 0.792406
4: 3447415.1: 0.876286 0.448215 0.791340
5: 3447413.5: 0.873344 0.445115 0.790446
6: 3447413.1: 0.874789 0.443935 0.789482
7: 3447412.9: 0.873407 0.443476 0.787969
8: 3447412.6: 0.874738 0.443452 0.786346
9: 3447399.6: 0.873381 0.435214 0.665693
10: 3447382.9: 0.873987 0.446658 0.545296
11: 3447380.0: 0.873637 0.440919 0.486841
12: 3447379.6: 0.874317 0.444942 0.472003
13: 3447379.5: 0.874401 0.443633 0.475912
14: 3447379.5: 0.874153 0.443656 0.475909
15: 3447379.5: 0.874185 0.443656 0.475662
16: 3447379.5: 0.874191 0.443667 0.475346
```

```
user  system elapsed
3237.977  28.393 3266.937
```
An initial model fit

Linear mixed-effects model fit by REML
Formula: gr.pt ~ (1 | id) + (1 | instr) + (1 | dept)
   Data: anon.grades.df
       AIC BIC logLik MLdeviance REMLdeviance
            3447387 3447437 -1723690 3447374 3447379
Random effects:
  Groups   Name   Variance  Std.Dev.
   id       0.3085   0.555
   instr    0.0795   0.282
   dept     0.0909   0.301
   Residual 0.4037   0.635
Number of obs: 1685394, groups: id, 54711; instr, 7915; dept, 102

Fixed effects:
       Estimate  Std. Error t value
   (Intercept)    3.1996      0.0314    102
How can such a computation be done?

- If we write a linear mixed model as
  \[ y = X\beta + Zb + \epsilon, \quad b \sim \mathcal{N}(0, \Sigma), \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I), \quad b \perp \epsilon \]  
  (1)
  where \( \Sigma \) depends on a parameter \( \theta \) (the three relative variance components, in the example), then \( Z \) and \( \Sigma \) are very sparse.
- Let \( \Sigma(\theta) = T(\theta)S(\theta)S(\theta)T'(\theta) \) be the “LDL” form of the Cholesky factorization of the relative variance matrix. That is, \( T \) is unit lower triangular and \( bmS \) is diagonal and on the scale of the relative standard deviation, not the variance. In our example \( T = I \).
- Let \( P \) represent the fill-reducing permutation for \( Z'Z \).
- For a given value of \( \theta \) set \( V = ZT(\theta)S(\theta)P' \).
The mixed model equations

- We work with the Choleksy decomposition of an extended system matrix

\[
\begin{bmatrix}
P(V'V + I)P' & PV'X & PV'y \\
X'VP' & X'X & X'y \\
y'VP' & y'X & y'y
\end{bmatrix} = R'R
\]  
(2)

where

\[
R = \begin{bmatrix}
L' & R_{VX} & r_{Vy} \\
0 & R_X & r_{Xy} \\
0 & 0 & r
\end{bmatrix}
\]  
(3)

- The matrices \(L'\) and \(R_X\) are upper triangular of dimension \(q \times q\) and \(p \times p\) respectively. The corresponding vectors, \(r_{Zy}\) and \(r_{Xy}\), are of dimension \(q\) and \(p\), and \(r\) is a scalar.
Profiled deviance functions

• The *profiled deviance* function

\[-2 \ell(\hat{\beta}(\theta), \theta, \hat{\sigma}^2(\theta)|y)\]

\[= n \log \left( \frac{2\pi r^2(\theta)}{n} \right) + n + 2 \log |L(\theta)|\]

\[= n [1 + \log (2\pi/n)] + n \log r^2(\theta) + 2 \log |L(\theta)|. \quad (4)\]

• The profiled REML deviance is

\[-2 \ell_R(\theta, \hat{\sigma}^2(\theta)|y)\]

\[= (n - p) [1 + \log (2\pi/(n - p))] + (n - p) \log r^2(\theta)\]

\[+ 2 \log |L(\theta)| + 2 \log |R_X(\theta)|. \quad (5)\]
An initial model fit

```r
> object.size(m1)/(2^20)
[1] 747.95

> slotsz(m1)/(2^20)

L    Vt    Zt    frame    flist    X
5.2332e+02 6.4294e+01 6.4294e+01 4.4384e+01 2.3057e+01 1.2859e+01
RVXy    ZtXy    uvec    ranef    call    terms
9.5734e-01 9.5734e-01 4.7861e-01 4.7861e-01 2.6398e-03 2.5024e-03
dims    deviance    cnames    fixef    RXy    XytXy
offset    weights
3.8147e-05 3.8147e-05
```
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- There are several approaches to dealing with large data sets in \textit{R}.
- The \texttt{fortune(122)} approach is generally not terribly successful.
- \textit{R} is not a filter (in the sense that SAS and SPSS are).
- At present the \texttt{model.matrix} function always outputs a full dense matrix. This is usually the point at which those working with large data sets run into trouble.
- It is possible, but not easy, to work with horizontal sections of the data and model matrix in the current formulation.
- The \texttt{lmer} function fits various types of mixed models using a sparse matrices but does not go through \texttt{model.matrix} for the sparse parts.
- The case of mixed models is somewhat special because grouping factors can be represented as indicators and you don’t need to watch for rank deficiencies.
- If both \( n \) and \( p \) are large (and if \( p \) grows with \( n \)) then mixed effects models are probably a good candidate.
- To fully realize the benefits of sparse matrix methods on the fixed-effects size, we should extend \texttt{model.matrix} to create a sparse matrix without any intermediate dense matrix.
- In some ways this is “back to the future” for some of us.