Regression Analysis of Proportion Outcomes with Random Effects

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Abstract

A regression method for proportional, or fractional, data with mixed effects is outlined, designed for analysis of datasets in which the outcomes have substantial weight at the bounds. In such cases a normal approximation is particularly unsuitable as it can result in incorrect inference. To resolve this problem, we employ a logistic regression model and then apply a bootstrap method to correct conservative confidence intervals. This paper outlines the theory of the method, and demonstrates its utility using simulated data. Working code for the R platform is provided through the package glmmboot, available on CRAN.

1 Introduction

Some processes yield bounded outcomes with heavy representation at the bounds. For example, if we consider the number of pages of a given issue of a magazine that are read by its subscribers, the distribution likely includes a large number of zeros (from those who didn’t have time to open the issue at all) and a large number at the maximum (from those who read cover to cover), and then some proportion spread in between. Or, to take a second example, a sampled person’s proportion of nights spent in a hospital in a given week must fall between zero and one, but among persons there will usually be vastly more zeros than anything else (most people aren’t hospitalized) and otherwise a disproportionate number of ones (some hospitalized people spend the whole week there, in longer-term care). Our paper discusses a technique for the analysis of such datasets in which the boundary values are common but don’t exhaust the set. Formally, we are interested in outcome data \( Y \in [0, 1] \), with many data points at the endpoints \( \{0, 1\} \). With trial-level covariates, we wish to model these data with regression, rather than collapsing to group means. Our covariates include both fixed effects and random effects.

If our outcomes were exclusively in \( \{0, 1\} \), we could for example run a straight-forward logistic regression with mixed effects. If our outcomes were strictly in \( (0, 1) \), we could consider a beta regression or similar methods. But these do not fit the problem at hand.

In the data we consider here, we do not feel that the zeroes and ones are conceptually different to the data within the interval. We would consider 0 and 0.01 almost the same. Similarly, seeing repeated measurements from a given input of \( y_1 = 0.8, y_2 = 1 \) would not be far from \( y_1 = 0.88, y_2 = 0.92 \). Thus we are averse to methods that fit separate covariates or models for the endpoint cases and the continuous cases, i.e. \( \{0, 1\} \) vs. \( (0, 1) \).

\(^1\) That is, the covariates are the same, \( x_1 = x_2 \)
2 Motivating Problem

While our method is more general than will be outlined in this section, we use this simple case to illustrate it.

2.1 Data Description

We consider outcome data of the form \( Y_i \in [0, 1] \), for \( i = 1, \ldots, n \), with a covariate of primary interest, \( X_i \in \{0, 1\} \), which can be thought of as a treatment indicator, along with fixed-effect covariates not of primary interest. Our data also contains a random effect \( Z_i \in \{1, 2, \ldots, K\} \). We could think of this for example as \( K \) participants each being measured over several trials.

2.2 Conditional Means

With the shorthand \( Y[x = 1] \) meaning the \( Y \) values for which \( X = 1 \), a typical conditional mean comparison would compare \( Y[x = 1] \) to \( Y[x = 0] \), i.e. comparing the means of each condition, with suitable standard deviations. Or we could do a comparison within the levels of our random effect, by comparing:

\[
\begin{align*}
Y[x = 1, z = 1] & \text{ vs } Y[x = 0, z = 1] \\
Y[x = 1, z = 2] & \text{ vs } Y[x = 0, z = 2] \\
& \quad \vdots \\
Y[x = 1, z = K] & \text{ vs } Y[x = 0, z = K]
\end{align*}
\]

(1)

And of course we can have multiple covariates of interest, which are not restricted to binary variables.

One problem with collapsing over trials as in the above is that we lose the ability to take trial-level predictors into account. Once we average over trials, we lose this small grain size in the predictors. This will affect our estimate of the effect of \( x \), and will not allow us to understand what role the other covariates play.

In the case of purely binary data, Dixon (2008) points out three further disadvantages of modelling constrained data in this way: if we wish to separate by some factor, we may have few observations in each condition, and the normal approximation could be inaccurate; due to the constraint, we may have floor or ceiling effects from averaging; and averaging artifacts can arise due to different numbers of observations across subjects or conditions. These arguments also apply to proportion data. Thus, we are seeking a method that allows us to retain the individual trial as the basic unit of the analysis, in spite of the fact that the trial-level outcomes are neither normal nor binary and therefore violate the assumptions of many familiar techniques.

3 Regression

The goal of regression is to model the expected value of \( Y_i \) as a function of our covariates \( x_i = (x_{i0}, x_{i1}, \ldots x_{ip})' \) to get \( E[Y_i \mid x_i] \). For now, for the sake of simplicity we will ignore random effects.
3.1 Linear Modelling

In a linear model, we assume the expected value of \( Y_i \) is a linear combination of the covariates, i.e. we have a vector \( \beta \) such that:

\[
E[Y_i \mid x_i, \beta] = x_{i0}\beta_0 + x_{i1}\beta_1 + \ldots + x_{ip}\beta_p = x'_i\beta
\]  
(2)

We can also think of this expectation not just as a linear combination of the covariates, \( x'_i\beta \), but as a function of this combination: the identity function \( I(x) = x \). That is, we can write:

\[
E[Y_i \mid x_i, \beta] = I(x'_i\beta) = x'_i\beta
\]  
(3)

This doesn’t change anything in this context, but using a function other than the identity would change the model.

Using a linear model with proportional outcomes raises many issues, similar to the problems that would be caused by using linear modelling with binomial \( Y \). Most directly, due to the bounding of \( Y \), we do not expect each covariate to affect the expected value of \( Y \) the same way for different baseline levels of \( E[Y] \); for example, when \( Y \) is expected to be large versus when it is expected to be close to \( \frac{1}{2} \). Similarly for an unbounded covariate \( x_j \), we don’t expect the effect of \( x_j \) on \( Y \) to remain the same for small and large values of \( x_j \). There is no guarantee that predictions will be contained in the interval \([0, 1]\), and the usual methods for fitting linear models assume the wrong error structure, especially for \( Y \) values near the boundaries.

3.2 Logistic Modelling

One way to fix these problems is to change the function of the linear combination of variables \( x'_i\beta \). Generalized linear models, or GLMs are one way to do this. GLMs are a flexible set of models that allow a large variety of outcome distributions.

Similar to \( (3) \), we’ll have:

\[
E[Y_i \mid x_i, \beta] = G(x'_i\beta)
\]  
(4)

with some function \( G(.) \) instead of the identity \( I(.) \) from before. We need \( G(x) \) to map to \((0, 1)\) and it should be increasing: as \( x'_i\beta \) increases, so does \( E[Y_i \mid x_i, \beta] \). \( G \) links the predictors to the mean. It is what is usually referred to as the inverse link function in the terminology of generalized linear modeling.

A common and often recommended choice of linking function is

\[
G(x) = \frac{e^x}{1 + e^x}
\]

This gives logistic regression. With binary \( Y \), this linking function has the interpretation of modelling the log odds as a linear combination of the covariates. While we don’t maintain that interpretation, we can still think of modelling proportion ratios instead of proportions:

\[
\log \left( \frac{E[Y_i \mid x_i, \beta]}{1 - E[Y_i \mid x_i, \beta]} \right) = x'_i\beta
\]  
(5)

\(^2\)Zero and 1 are excluded because \( Y \) would never have an expected value equal to either of the boundary values.
By employing the logistic function, we remedy the problem of ceiling effects. For example, an expected value for \( Y \) of 0.99 is as “far” from 0.95 as 0.95 is from 0.78. This method forms the basis of the method from Papke and Wooldridge (1996) to model \( Y \in [0, 1] \).

### 3.3 Quasi-Likelihood Methods

In the binary case of logistic regression, \( \mathbb{E}[Y] = P(Y = 1) \cdot 1 + P(Y = 0) \cdot 0 = P(Y = 1) \), directly modelling the probability of \( Y \). This makes solving for \( \beta \) simple, because we have the full distribution of the data, and therefore the likelihood. We generally solve for \( \beta \) by maximising the log likelihood \( l(b) \):

\[
l(b) = \sum_i \log P(Y_i = y_i | \beta = b, x_i)
\]

\[
= \sum_i l_i(b) \tag{6}
\]

We can use (4) to write:

\[
l_i(b) = y_i \log [G(x_i' b)] + (1 - y_i) \log [1 - G(x_i' b)] \tag{7}
\]

Full details are given in appendix A.

We note that above log likelihood function can be evaluated with \( y_i \in [0, 1] \), not just for \( \{0, 1\} \). It functions as linear interpolation between the 0 and 1 cases. This is no longer a true likelihood, but a true likelihood is not required to find a consistent estimate of \( \beta \). From Gourieroux, Monfort, and Trognon (1984), we only need (4).

We maximise the full quasi-log likelihood and thus we find the parameter vector that best fits the expected proportion \( Y \) given our predictors. The result is analogous to the outcome of an ordinary logistic regression. Even though the outcome being modeled does not fall only into values of zero and one, we still find the best fit for the expected value.

### 3.4 Interpreting Logistic Models

Interpretation of logistic models is less transparent than interpretation of linear models. Let us assume we have fit our model and have estimated \( \hat{\beta} \) as our best-fitting parameter vector; and assume further we also have confidence intervals and \( p \)-values.

Because the logistic is still a monotonic fit in our covariates, we can continue to interpret a highly significant variable as meaning the associated covariate is correlated with \( Y \). For example, if \( \beta_2 > 0 \), i.e. significantly above zero (with appropriately small \( p \)-value), we know that \( x_2 \) is positively correlated with \( Y \). That is, as \( x_2 \) increases, our expected value for \( Y \) will increase, and we are confident this is a significant pattern. This is the most fundamental and important interpretation.

\(^3\)This property of the logistic transform is effective in keeping predictions within bounds, but whether it is appropriate in considering the real-world domain of the analysis is important for the modeller to bear in mind. There may be domains in which a change from 50% to 55% is, in fact, the same as a change from 90% to 95% in how the predictors influence outcomes. This is a question that could be addressed empirically, but is not one that we evaluate here.
The direct rate of change using the derivative is:

\[
\frac{\partial}{\partial x_j} \mathbb{E}[Y \mid x, \beta] = \beta_j \frac{\exp(x_i'\beta)}{(\exp(x_i'\beta) + 1)^2}
\]  

(8)

This can be used for any specific \( x \), but is not easy to interpret as-is. One simplification is that near the midpoint, i.e. when \( \mathbb{E}[Y \mid x, \beta] \) is close to \( \frac{1}{2} \), this derivative will be approximately \( \beta_j/4 \). So if \( \beta_3 = 0.2 \), then a unit increase in \( x_3 \) will increase the expected proportion by approximately 0.05. This interpretation only works for small changes in \( x \) and/or small values of \( \beta_3 \). When the predictions are close to zero or one, where the nonlinearity of the logistic linking function becomes more important, the effects of a change in a variable on the mean of \( Y \) will be smaller.

As mentioned in the prior section, in the binary case of logistic regression we can interpret our coefficients in terms of odds: the ratio of the probability of \( Y = 1 \) over the probability of \( Y = 0 \). Instead of probabilities, we interpret our coefficients in terms of proportion ratios. For example, if we’re measuring the proportion of time a football team has possession of the ball, an expected proportion of 0.75 is equivalent to expecting that team to have the ball three times as much as the opposition, \( \frac{3}{2} \).

Letting \( \hat{\text{prop}}_i \) be the expected proportion in trial \( i \), and exponentiating both sides of (5), we can write:

\[
\hat{\text{ratio}}_i = \frac{\hat{\text{prop}}_i}{1 - \hat{\text{prop}}_i} = \exp(x_i'\hat{\beta})
\]  

(9)

To understand what happens when we change a value of \( x \), let \( x_i^{\text{old}} \) be a vector of covariates. Assume we increase \( x_3 \) by 1, to get \( x_i^{\text{new}} \). These covariates, new and old, give different expected ratios, \( \hat{\text{ratio}}_i^{\text{new}} \) and \( \hat{\text{ratio}}_i^{\text{old}} \). We can look at how the ratios will change. First note that \( (x_i^{\text{new}})'\hat{\beta} = (x_i^{\text{old}})'(\hat{\beta} + \hat{\beta}_3) \), since we increase \( x_3 \) and leave the rest.

\[
\frac{\hat{\text{ratio}}_i^{\text{new}}}{\hat{\text{ratio}}_i^{\text{old}}} = \frac{\exp((x_i^{\text{new}})'\hat{\beta})}{\exp((x_i^{\text{old}})'\hat{\beta})}
\]

\[
= \frac{\exp((x_i^{\text{old}})'(\hat{\beta} + \hat{\beta}_3))}{\exp((x_i^{\text{old}})'\hat{\beta})}
\]

\[
= \frac{\exp((x_i^{\text{old}})'\hat{\beta})\exp(\hat{\beta}_3)}{\exp((x_i^{\text{old}})'\hat{\beta})}
\]

\[
= \exp(\hat{\beta}_3)
\]  

(10)

Thus we have an interpretation of \( \exp(\beta_j) \) as the multiplicative change in the ratio of proportions. Going back to the sports analogy, imagine that ball possession is affected by how much rain fell before the match. Suppose our coefficient for rainfall (in mm) was 0.4. An extra mm of rain would increase the ratio by a factor of \( \exp(0.4) \approx 1.5 \). So if our team had been expecting 30% possession with 1 mm of rain, a ratio of \( \frac{3}{7} \), they expect 1.5 times this with 2 mm of rain, or a ratio of 0.64. This corresponds to 39% possession.

Appendix B offers interpretations when \( \mathbb{E}[Y \mid x, \beta] \) is close to the endpoints.
3.5 Random Effects

The preceding examples assumed relatively simple models, but for many practical applications mixed-effects modeling is more appropriate. Once mixed effects are considered, \( \mathbb{E}[Y \mid x, \beta] = G(x'\beta) \) is no longer true. A typical mixed effects model adds a design vector \( z \) and a random vector \( B \). The design vector is fixed. It can represent, for example, a vector containing a unique identifier for each participant in a study, while the random vector represents the variation from the random effects. When adding random effects, we can make a similar statement about the conditional distribution of \( Y \) given \( B = b \):

\[
\mathbb{E}[Y \mid x, \beta, z, B = b] = G(x'\beta + z'b)
\]

(11)

with \( B \sim \mathcal{N}(0, \Sigma) \), a normal distribution with unknown variance. The expected value of \( Y \) without the unknown random vector is the average value over the distribution of \( B \):

\[
\mathbb{E}[Y \mid x, \beta] = \int_B G(x'\beta + z'b)f(b) \, db
\]

(12)

where \( f(.) \) is the pdf of \( B \). See Bolker et al. [2009] for details.

For a given realization of random effects, i.e. a fixed but unknown vector \( b \) such that \( B = b \), the conditional interpretations already discussed are valid. For example, say we want subject-level random effects (i.e. random intercepts). For a specific subject, we can interpret the effects of \( x \) as in the prior subsection.

3.6 Summary

In summary, to run a regression method on outcomes in \([0, 1]\) with trial-level covariates, we run a quasi-likelihood version of logistic regression: we keep the interpretation of fitting the mean, but no longer assume we’re specifying the whole distribution - in particular we don’t need to specify the variance. On top of this, we add random effects, for appropriately modelling many practical applications. In section 5 we will describe current statistical software for fitting such models.

In some cases, no more needs to be added. A small change in model specification allows non-binary models to be fit by methods traditionally associated with binary data, with consistent parameter estimation and valid standard errors. However, these models are conservative. We discuss the issue and a remedy in the following section.

4 Variance Correction

Nearly all estimation methods for the parameter vector will also produce standard errors. The specific calculation will depend on the software implementation, but generally the standard errors will be generated with respect to the nominal likelihood. For example, if we assume a logistic link function for our quasi-likelihood fit, we may be given standard errors generated from that functional form.

We only wish to specify the conditional mean of our data, not the variance, thus we don’t want to put any assumptions on the variance. Further, typical implementations for proportion or fractional data can be conservative, i.e. the standard errors will be too large. This

\footnote{Note that \( B \) and \( \beta \) are not the same}
is partially due to the standard errors being estimated assuming the worst case scenario, in which the variance of $Y$ given $x$ is $\nu(1 - \nu)$, where $\nu = E[Y \mid x, \beta]$. This is the correct specification for binary $Y$, while proportional $Y$ has less variance on average, and thus more accuracy.

4.1 Correction Methods

There are three main ways to correct the variance estimates. The first is by using sandwich estimators, also known as heteroscedasticity-consistent standard errors (White 1980). Papke and Wooldridge (1996) use sandwich estimators. We don’t use these because we don’t wish to rely on asymptotics - there is no guarantee that such asymptotics will converge in a reasonable time, especially if any skewness is present. In our simulations, sandwich methods seemed to be conservative.

Secondly, we can use over-dispersion methods (McCullagh 1984 page 124). These are hard to specify with random effects, and rely on the functional form of the mean $5$, so we don’t use these.

Finally, we can use bootstrap methods, which we will describe further in the following sections.

4.2 Bootstrap Method

Bootstrapping is a resampling technique that uses resampling with replacement. In inference, we’re trying to use information from our sample, i.e. our original data, to infer details about the population. We can approximate this relationship by treating our sample as a population, and letting our resamples act as samples from it. In other words, our resamples are to our sample as our sample is to our population.

Consider, for example, estimating the variance of a coefficient. A given regression analysis over a sample from a population will yield a coefficient specifying the influence of each predictor. This coefficient may be the closest estimate for the analyzed sample, but it would be good to have an idea of how representative that coefficient is over the whole set of samples we could have randomly drawn from the same population. We can simulate this process of having more than one sample by bootstrapping. We resample our data with replacement multiple times, and estimate the coefficient for each resampled data set. We then use the variance of these resampled coefficients as our variance estimate for the sample.

For the quasi-likelihood method outlined in section 3.3 we work with the assumption outlined in $4$, i.e. that we’re fitting the expected value of $Y$. We fit this quasi-likelihood method assuming $G$ is the logistic function. As discussed, this implies a variance structure on $\beta$, but we might not trust that this process will generate correctly specified $t$ distributions for inference. In particular, because binary data generally presents greater variance than the continuous data we are contemplating here, there is a risk that the $t$ distributions will yield overly conservative inference, and thus less power.

$5$That is, the relationship between the inputs and the mean.
4.3 Bootstrap Resampling with Random Effects

Ordinary bootstrap resampling is simple: resample each row with replacement, with equal weight. When random effects are included in a model, we can no longer resample in such a straightforward manner. Instead, we have to simulate the data-generating process as closely as possible. We do this by block resampling (McCullagh 2000): we resample from blocks with replacement, where the blocks are defined by the random effects.

For example, with subjects as our random effect, we resample subjects with replacement. Every time a subject is selected, we select all their observations, without replacement. McCullagh (2000) shows that resampling a second time within the blocks is conservative and unnecessary.

With one random effect, the above is well-defined. With two or more, a valid resampling procedure becomes more difficult to define. We discuss in appendix C how to implement methods from Owen and Eckles (2012) if desired.

4.4 Bootstrapping One Random Effect, not Multiple

In practice, we don’t use multiway bootstrap methods: they are generally even more conservative than using the implied binary variance structure, i.e. the raw model output from running the proportional models in most statistical software.

Thus, in our analysis pipeline we enter all appropriate random effects into the original model; then, when using bootstrapping to estimate the variance of the coefficients, the bootstraps only include one of the random effects. Bakshy and Eckles (2013) show that taking into account only one type of dependence structure, or random effect, gives valid inference under the typical null hypothesis, even without building a model with random effects. In our simulation examples, taking only one random effect into account on the level of the bootstrap retains correct (or conservative) coverage.

As we discuss in our simulation study, we bootstrap over the random effect that has more levels because the coverage of our intervals is much better with more levels.

4.5 Generating Bootstrap Results

Once we’ve chosen what level we’re resampling with replacement from, we resample $R$ times for some large $R$ and refit our model on each new dataset. This generates a set of parameter vectors, $\hat{\beta}_1^*, \hat{\beta}_2^*, \ldots, \hat{\beta}_R^*$, along with standard error vectors from each bootstrap, which we’ll call $\hat{se}_{\hat{\beta}_j}$, for $j = 1, \ldots, R$. From our regression on the full original dataset, which we’ll call the base regression, we have $\hat{\beta}$ and $\hat{se}_{\beta}$.

Note also that our bootstrap methods are non-parametric: we resample blocks of trials and refit our model on the resampled data, rather than resampling residuals. The alternatives, bootstrapping residuals, are difficult to justify since we don’t specify a model, only a mean structure. With our non-parametric bootstrap, we must be wary of small-sample problems with discrete covarites.

It is non-trivial to generate confidence intervals and p-values from bootstrap estimates. We...
follow Hesterberg (2015) in using our bootstrap samples to approximate the distribution of
the “t” values produced by our regression, from Efron and Tibshirani (1994). This statistic is
a pivotal quantity: it does not depend on unknown parameters, such as the model variance.

Suppose that we’re interested in the jth covariate parameter, $\beta^j$. We have the estimate $\hat{\beta}^j$, and the standard error $\hat{se}_{\beta^j}$ from our base regression. (For now, we drop the $j$ notation.) In testing against zero, we typically generate:

$$t_{\text{plain}} = \frac{\hat{\beta} - 0}{\hat{se}_{\beta}}$$

(13)

Under any issues outlined in section 4.2 we might not believe that this statistic will actually have a t distribution. Instead of assuming a distribution on this statistic, we use our bootstrap samples to estimate the distribution: we generate the $R$ bootstrap t statistics in the same way as we do in the base regression:

$$t^* = \frac{\hat{\beta}^* - \hat{\beta}}{\hat{se}_{\beta^*}}$$

(14)

Letting $q_\alpha$ be the $\alpha$ quantile of the bootstrap t distribution, the interval is then:

$$(\hat{\beta} - q_{1-\alpha/2}\hat{se}_{\beta}, \hat{\beta} - q_{\alpha/2}\hat{se}_{\beta})$$

(15)

Just as with any confidence intervals from regression, we can reject e.g. zero at level $\alpha$. We can turn this around to form p-values: we calculate the largest $\alpha$ such that this interval contains zero.

### 4.6 Confidence Intervals and p-values for Random Effects

Non-pivotal bootstrap methods can suffer from two sources of narrowness. They come from the equivalent of using $z$ instead of $t$, and from dividing the sample standard deviation by $\sqrt{n}$ instead of $\sqrt{n-df}$ to get standard errors. The bootstrap $t$ method from the previous section in theory does not suffer from these bootstrap issues, since it directly estimates the $t$-distribution, specifically the $t$-distribution with the correct degrees of freedom.

Many statisticians who are well-versed in random effects modeling are wary of constructing p-values for models with random effects; see for example Baayen, Davidson, and Bates (2008). We are similarly cautious. Our bootstrap method is capable of providing p-values if desired, warnings notwithstanding.

See the next section for advice about interpreting p-values less than 0.05.

### 4.7 Practical Considerations for Bootstrapping

Hesterberg (2015) recommends $R > 15,000$ for published works, and we agree.

If time is a concern, and e.g. model-fitting is slow for a given problem, doing 15,000 runs multiple times may not be feasible. For small-scale model checking, the standard errors straight from the base regression are likely to give an acceptable first approximation. Of course these multiple models should not be guiding your decision of model selection.

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7 Not strictly true in random effect models, but the difference is small enough to not matter.
In terms of the $p$-values: this large $R$ is recommended because it gives reasonable guarantees about accuracy near the typical 0.025 quantile points. If we’re estimating a smaller $p$-value than 0.05, and are therefore outside of the 0.025 bound on either side, our accuracy will be lower, and our $p$-value estimate will be subject to greater random noise due to resampling for the bootstrap. This is because we are estimating the $p$ value by counting how often a rare event occurs. The number of sample draws thus has to be very large to accurately estimate the long tails of the probability distribution. Intuitively, you cannot accurately judge the actual probability of a one-in-a-hundred event by looking at a hundred samples, or a thousand; as we walk down the tail of the distribution, the granularity of the bootstraps overwhelms their accuracy. We therefore advocate against taking $p$-values below 0.05 as being informative. If the researcher is particularly interested in a threshold below 0.05, Hesterberg (2015) provides the calculation for how many resamples gives acceptable accuracy. In any case, using miniscule $p$ values as shorthand for strong effects is contraindicated as a general matter, not just for bootstrapping analyses (see for example Sullivan and Feinn (2012)), but this practice carries additional risks in bootstrap analyses.

5 Work Flow

Before we bootstrap, we need an algorithm capable of solving the quasi general mixed model from (12). We use the glmmTMB R package (Magnusson et al. 2017). For those familiar with the R package lme4, the notation is the same.

While this package does not contain an equivalent of the glm function’s quasibinomial distribution family, we can run it with the standard binomial family input (with default logistic link). This gives us the solution under equation (4) as desired, although with conservative standard errors referred to in section 4.2.

Once the practitioner is satisfied that her model runs as desired in glmmTMB, she can use the bootstrap to generate confidence intervals and $p$-values for the parameters in her model. We call the model run on the original data the “base model”. Code for the following work is provided on CRAN, at https://cran.r-project.org/web/packages/glmmboot.

The number of bootstrap resamples, $R$, is set to some reasonable choice (~15,000 per Hesterberg). For each sample, a resampling of the random effects is generated as in section 4.3 which generates a full resampled data set. The model is then run exactly as in the base model on this resampled data set. The output is saved, i.e. estimates and standard errors from each bootstrap run. This is by far the longest step in terms of computation time. Once these are run and saved, all bootstrap output plus the output from the base model are combined to form produce corrected confidence intervals and $p$-values, using the bootstrap $t$ method, from section 4.5.

5.1 Recommended Output

Our next task is to produce overall output from the method, i.e. the result of the full work flow from above.

We don’t recommend using the bootstrap to adjust the base model’s parameter estimates, $\hat{\beta}$. This is the most important model output, and its value and interpretation does not depend on bootstrap output. We do recommend reporting the bootstrap confidence intervals. The bootstrap $p$-values are usually of interest too.
An optional but interpretable output is the standard errors from the base model. Since these are generally conservative and are independent of the bootstrap, they provide a grounding for significance results from the bootstrap, as well as a quick indication of how much less conservative the bootstrap approach is. Further, the bootstrap CIs are not necessarily symmetric around the estimates, so these unadjusted standard errors can be useful for a quick symmetric estimate of variability.

6 Simulation Study

We run a factorial simulation study over multiple parameters including the number of rows, 1000 and 2000; the number of fixed effect parameters (not including the intercept), 3 and 10; the number of random effects, one or two; crossed and uncrossed random effects; correlated and uncorrelated parameters. Further, we vary the number of levels of each random effect, either 10, 20, 40 or 80. In half our simulations, we use zero fixed effects, and random non-zero effects in the other half.

We generate a random vector \( B \) from a normal distribution. The known design matrix \( X \) is generated according to a mixture of a randomly correlated multivariate normal distribution and independent uniform random variables. When the fixed effects are non-null, we generate normal random fixed effects.

The mean vector is then fit according to equation (11), and finally \( Y \) is generated in one of two ways. Mostly, we generated from a beta distribution, with the parameters set to:

\[
\begin{align*}
\alpha &= \mu^2 (1 - \mu) \sigma^{-2} \mu \\
\beta &= \alpha (\mu^{-1} - 1)
\end{align*}
\]  

(16)

\( \mu \) is from the mean vector. We set \( \sigma^2 \) to be \( \rho^2 \mu (1 - \mu) \), with \( \rho \in (0, 1) \). As \( \rho \to 1 \), the beta distribution essentially produces binary data with \( p = \frac{\mu}{2} \) smaller values of \( \rho \) produce more values within the interval \((0, 1)\). This sets the mean and variance of the beta distribution to \( \mu \) and \( \sigma^2 \) respectively. Alternatively, we generate uniform noise bounded to keep \( Y \) in the unit interval.

For each simulated model, we also run an “oracle” model: we enter the random vector \( B \) into this model as a fixed predictor. This allows us to fit the model with the \texttt{glm} function’s \texttt{quasibinomial} distribution family, from \texttt{R}.

6.1 Type I Errors

Our primary interest is verifying correct type I coverage. That is, if the true effect is zero, our 95% confidence intervals should cover zero at least 95% of the time.

We first plot the results with a single random effect. Figure 1 plots the type I error against the number of levels in the random effect, both overall in green, and separated by number of parameters in the model in yellow and red, for ten and three parameters respectively. The light blue regions are the 95% prediction intervals under the null; the inner regions for the overall result, and the outer for the separated results.

---

8Note that with \( \rho < 1 \), the beta distribution can still produce near boundary values, i.e. values arbitrarily close to zero and one. If at least one of \( \alpha \) or \( \beta \) is less than one, this can occur.

9Larger region due to lower counts.
ten-parameter effects than three. Finally, we add the coverage rates of the base model confidence interval in black.

![Figure 1: Type I error by number of levels in the random effect. Green points are overall coverage for that level, yellow are for three-parameter models and red for the ten-parameter models. The black points below are from the base model.](image)

In general, these results are good. Only one result stands out as poor: when we have ten levels and ten fixed effects, not including the intercept. This is a difficult case for any non-linear model. Once we reduce our model to just three fixed effects beyond the intercept, even with ten levels in the random effect we get correct coverage.

In contrast, the base model is very conservative, rejecting only about 2% of the time from a nominal 5%.

Figure 2 shows the results for two random effects. While we bootstrap the effect with more levels, the effect with fewer levels has a stronger effect on coverage. Thus we plot coverage against the smaller of the two level counts. From there, the only major difference relative to the first plot is that the number of elements to check is not the same at each level.

The results are good here too - for all level counts except ten, all coverage intervals are within their 95% null intervals. And again, the base intervals are generally quite conservative.

### 6.2 Relative Interval Length

It’s worth seeing how the interval widths of the bootstrapped intervals compare to the base interval widths. Recall above we control the standard deviation of Y with a parameter \( \rho \), and as \( \rho \to 1 \), we get binary data; smaller values of \( \rho \) give more values near the expected
Figure 2: Type I error by number of levels in the random effect. Green points are overall coverage for that level, yellow are for three-parameter models and red for the ten-parameter models. The black points below are from the base model.

mean of $Y$. Thus we plot the relative width of the intervals, i.e. bootstrap width divided by base width, against the parameter $\rho$.

Figure 3 plots the ratio of bootstrap width divided by base width against the values of $\rho$ we use in our study. We fit a smooth spline, in gold, and the line of equality $y = x$, in green, and we add the line $y = 1$ in blue for comparison.

The smooth spline, with five degrees of freedom, is nearly linear and the line is just below the line of equality. This suggest that on average, the bootstrap is doing the right thing: it scales the length of the intervals down by the same amount the standard deviation of the $Y$ values are relative to the binary case. In fact, it’s smaller than that, as we can see with the fit line below the line of equality everywhere.

Note that this could give a shorthand method of getting confidence intervals from regression methods: just scale down the width of the interval by $\rho$. Unfortunately, we don’t know $\rho$; seeing boundary values could mean the expected value of $Y$ was close to zero and the standard deviation was small, or it could be a moderate expected $Y$ and a large $\rho$. Further, there won’t be a fixed $\rho$ for real data.

7 Conclusion

We have presented a method for analyzing bounded continuous outcome data in which outcomes near the bounds are frequent, but data within the range are also common. Under
such conditions simply performing an ordinary linear regression is inappropriate because such analyses presuppose normally distributed error terms, resulting in potentially biased inference. Another common technique, that of collapsing outcomes over some grouping variable (such as subject and condition), is not wrong in and of itself, but it may be underpowered, as it excludes entering trial-level predictors into the model, and suffers other defects as indicated above. The present procedure avoids these problems.

The primary costs to implementing the present method are that (a) the outcomes are presented in possibly unfamiliar units, and (b) bootstrapping to give precision to the confidence intervals demands a more substantial set of computations. To manage (a), we recommend providing explicit examples in the description of the model. For example, the regression output table should include not only the $\beta$ coefficients, but also their exponent, perhaps accompanied by an illustrative example given in the text (e.g., “$\exp(\beta)$ estimates the multiplicative change in the ratio of outcome $a$ to outcome $b$ given a one-unit increase in [that variable].” followed by a specific numerical example). Readers familiar with logistic regression will already be familiar with interpretation of odds ratios, but others might not.

Managing the computing requirements of the bootstrap analyses depends on the researcher’s computing resources, but note that in a normal analysis pipeline the bootstrapping analysis will generally follow model exploration; that is, establishing definitive confidence intervals comes after most of the analysis work is done. This minimizes the practical costs of implementing the procedure, with the benefit of less conservative inference.

Code for the R platform, together with illustrative examples, is available through the Comprehensive R Archive Network (CRAN), at
https://cran.r-project.org/web/packages/glmmboot.
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A Logistic Log Likelihood

Note again that in the binary case, we have $E[Y] = P(Y = 1) \cdot 1 + P(Y = 0) \cdot 0 = P(Y = 1)$, This makes solving for $\beta$ straight-forward, since we have the full distribution of the data, and therefore the likelihood.

We can also write this probability in terms of any given $y$. Raising any number to the power 1 leaves it unchanged, and raising any nonzero number to the power zero gives unity, thus we can write:

$$P(Y = y | x) = P(Y = 1 | x)^y \times P(Y = 0 | x)^{1-y} =$$

(17)

Checking the two cases, $y = 1$ and $y = 0$, shows the equality.

We want to write the likelihood using this. Likelihood of the data is $L(\beta | y, x) = P(Y = y | \beta, x)$. For one trial, this is:

$$L(b | y_i, x_i) = P(Y = y_i | \beta, x_i)$$

In words, the likelihood of a parameter vector given the data is the probability of the data given that parameter vector, with both conditional on the predictors $X$.

The parameters that maximize the log likelihood are the same parameters that maximize the likelihood. The log-likelihood is easier to maximize, since it turns products into sums, thus we work with the log likelihood. Let $l(\beta | y) = \log L(\beta | y)$ be the log likelihood. To keep our notation easier, let $L_i(b) = L(b | y_i, x_i)$ and $l_i(b) = \log L_i(b)$ and we’ll drop writing $x_i$ wherever it’s implied.

Using (17), we can write:

$$L_i(b) = P(Y = 1 | b)^{y_i} (1 - P(Y = 1 | b))^{1-y_i}$$

To reiterate, this just means:

$$L_i(b) = \begin{cases} P(Y = 1 | b) & \text{if } y_i = 1 \\ P(Y = 0 | b) & \text{if } y_i = 0 \end{cases}$$

(18)

Using (17), we can then write:

$$L_i(b) = G(x'_i b)^{y_i} (1 - G(x'_i b))^{1-y_i}$$

(19)

Similarly for the log likelihood, we write:

$$l_i(b) = \log(P(Y = y_i | b))$$

(20)

$$= \log(P(Y = 1 | b)^{y_i} (1 - P(Y = 1 | b))^{1-y_i})$$

$$= y_i \log[P(Y = 1 | b)] + (1 - y_i) \log[1 - P(Y = 1 | b)]$$

(21)
Going through both cases, we can again see that this is simply:

\[
\begin{align*}
\log[P(Y = 1 \mid \beta = b)] & \quad \text{if } y_i = 1 \\
\log[P(Y = 0 \mid \beta = b)] & \quad \text{if } y_i = 0
\end{align*}
\]  

(22)

We again use (14) to write:

\[
l_i(b) = y_i \log[G(x_i'b)] + (1 - y_i) \log[1 - G(x_i'b)]
\]  

(23)

However, the above log likelihood function can be evaluated with \(y_i \in [0, 1]\), not just for \(\{0, 1\}\). We lose the direct interpretation of equations (18) and (22), but plugging any \(y_i \in [0, 1]\) in for equation (23) shows that we now have a linear interpolation between the 0 and 1 cases from (22). This is no longer a true likelihood, but that is not required to find a consistent estimate of \(\beta\), while assuming (4).

From here, we maximise the full quasi-log likelihood \(L(b) = \prod_i l_i(b)\), and thus we find the parameter vector that best fits the expected proportion \(Y\) given our predictors.

### B Further Logistic Interpretations: Endpoints

When the ratios are very small, the ratio of ratios will be very close to the ratio of proportions. For example, assume we have two proportions \(1/50\) and \(3/100\). The ratio of proportions will be \(1/50 \div 3/100 = 1/50 \times 100/3 = 100/150 = 2/3\), or \(\approx 0.667\).

Converting the proportions to ratios gives 1:49 and 3:97; dividing these as fractions produces \(1/49 \div 3/97\), or \(97/49 \times 3\) or \(\approx 0.660\). Thus, arithmetically the difference between comparing proportions, and comparing ratios, is small when both ratios are small themselves.

For an example when this approximation doesn’t work, assume we have two proportions \(3/4\) and \(1/5\). The ratio of proportions will be \(15/4 = 3.75\). Converting the proportions to ratios gives 3 and \(1/4\) respectively, and thus the ratio of ratios is 12, not that close to 3.75.

This is an arithmetic consequence of the relationship between ratios and proportions. Thus, with \(E[Y \mid x]\) close to zero, a unit change in \(x_j\) can be interpreted as:

\[
\frac{\text{prop}_{\text{new}}}{\text{prop}_{\text{old}}} \approx \exp(\hat{\beta}_j)
\]  

(24)

A bad team with expected possession of 5% would expect their proportion to increase by a factor of \(\exp(0.4) = 1.5\) with a one mm increase in rainfall, to get to 7.5%. This is close to the true value of 7.3%.

Similarly, when \(E[Y \mid x]\) is close to one, i.e. large ratios, we can interpret

\[
\frac{1 - \text{prop}_{\text{new}}}{1 - \text{prop}_{\text{old}}} \approx \exp(-\hat{\beta}_j)
\]  

(25)

Now a great team with expected possession of 90% would expect their proportion of not having possession to decrease by a factor of \(\exp(-0.4) = 2/3\), down to 6.7% from 10%. This is close to the true value of 7%.

Note that for the ratios interpretation, there is no approximation required.
Figure 4: Our original data counts are on the left, and counts from a resampled data set are on the right. Matching colors are example cases of matched data counts.

C Multiple Random Effects

We first discuss two random effects, which can be independent or crossed.

McCullagh (2000) shows that no resampling method exists that gives the correct variance estimate for crossed random effects. However, Owen and Eckles (2012) outline methods that are conservative and therefore valid, and are only mildly conservative in most cases. We focus on the simpler method for two Owen (2007) pigeonhole bootstrap. With multiple uncrossed effects, this method should be close to unbiased.

We consider our data as a two-way random array, in that we have two factors, i.e. two random factors over which we intend to generalize the results of the model. We sample each factor independently: within each factor, we resample with replacement, with equal probability, to get a sample size that matches our data. For example, suppose we have a dataset that comes from a set of human participants who respond to a series of trials, where each trial makes use of one item from a small set of items. If we have $n$ trials, $K$ participants and $L$ items (with $K, L < n$), a full resample of participants would be a sample of size $K$, with each one randomly sampled from the population of $K$ participants. For any given bootstrap resample, we are very likely to have some datapoints not show up while others do so multiple times.

If participant $i$ shows up $A$ times in a given resample, and item $j$ shows up $B$ times, we take all rows with participant $i$ and item $j$ $AB$ times. There may be no rows with this combination, or there could be many. If for example participant $i$ is sampled twice, item $j$ is sampled three times, and there are five rows in the original dataset with participant $i$ and item $j$, then this particular resample will pick up each of those rows six times, for a total of $30$ rows with that participant-item combination.

Figure 4 shows an example: our original data are on the left, with a series of participants (named columns) responding to a set of words (rows). We resample over items with replacement, and over participants with replacement, to get our resampled data on the right. Since data are resampled with replacement, we get some items and participants showing up more than once, and some never. If a pairing doesn’t have any data in our original array, such as (Ball, Chris), then there are no rows included for that pairing in our resampled data either.
When we sample with replacement, each original value is selected at least once with approximately a $0.63 = 1 - e^{-1}$ chance. With a two-dimensional array, each pair is selected at least once with an approximately $0.4 = (1 - e^{-1})^2$ chance.