Maximum likelihood estimation and analysis with the bbmle package

Ben Bolker

March 13, 2011

Contents

| 1 | Exa | mple: | Orobanche/overdispersed binomial | 2 | | | | | | | | |
|---|-------------|---------|---|------|--|--|--|--|--|--|--|--|
| | 1.1 | Test b | pasic fit to simulated beta-binomial data | . 2 | | | | | | | | |
| | 1.2 | Real | data (<i>Orobanche</i> , Crowder (1978)) | . 5 | | | | | | | | |
| 2 | Exa | mple: | reed frog size predation | 11 | | | | | | | | |
| 3 | Newer stuff | | | | | | | | | | | |
| 4 | Tec | hnical | details | 15 | | | | | | | | |
| | 4.1 | Profili | ing and confidence intervals | . 15 | | | | | | | | |
| | | 4.1.1 | Estimating standard error | . 15 | | | | | | | | |
| | | 4.1.2 | Profiling | . 16 | | | | | | | | |
| | | 4.1.3 | Confidence intervals | . 17 | | | | | | | | |
| | | 4.1.4 | Profile plotting | . 18 | | | | | | | | |
| | | | | | | | | | | | | |

Note: I have suppressed the continuation character (+) in the R examples throughout this document, as I find it easier to read/cut-and-paste where necessary.

The bbmle package, designed to simplify maximum likelihood estimation and analysis in R, extends and modifies the mle function and class in the stats4 package that comes with R by default. mle is in turn a wrapper around the optim function in base R. The maximum-likelihood-estimation function and class in bbmle are both called mle2, to avoid confusion and conflict with the original functions in the stats4 package. The major differences between mle and mle2 are:

- mle2 is more robust, with additional warnings (e.g. if the Hessian can't be computed by finite differences, mle2 returns a fit with a missing Hessian rather than stopping with an error)
- mle2 uses a data argument to allow different data to be passed to the negative log-likelihood function

- mle2 has a formula interface like that of (e.g.) gls in the nlme package. For relatively simple models the formula for the maximum likelihood can be written in-line, rather than defining a negative log-likelihood function. The formula interface also simplifies fitting models with categorical variables. Models fitted using the formula interface also have applicable predict and simulate methods.
- bbmle defines anova, AIC, AICc, and BIC methods for mle2 objects, as well as AICtab, BICtab, AICctab functions for producing summary tables of information criteria for a set of models.

Other packages with similar functionality (extending GLMs in various ways) are $\,$

- on CRAN: aod (overdispersed models such as beta-binomial); vgam (a wide range of models); betareg (beta regression); pscl (zero-inflated, hurdle models); maxLik (another general-purpose maximizer, with a different selection of optimizers)
- In Jim Lindsey's code repository (http://popgen.unimaas.nl/~jlindsey/rcode.html): gnlr and gnlr3

1 Example: Orobanche/overdispersed binomial

This example will use the classic data set on *Orobanche* germination from Crowder (1978) (you can also use glm(...,family="quasibinomial") or the aod package to analyze these data).

1.1 Test basic fit to simulated beta-binomial data

First, generate a single beta-binomially distributed set of points as a simple test. Load the emdbook package to get functions for the beta-binomial distribution (random-deviate function rbetabinom — these functions are also available in Jim Lindsey's rmutil package).

> library(emdbook)

Generate random deviates from a random beta-binomial:

```
> set.seed(1001)
> x1 = rbetabinom(n=1000,prob=0.1,size=50,theta=10)
Load the package:
```

> library(bbmle)

Construct a simple negative log-likelihood function:

The summary method for mle2 objects shows the parameters; approximate standard errors (based on quadratic approximation to the curvature at the maximum likelihood estimate); and a test of the parameter difference from zero based on this standard error and on an assumption that the likelihood surface is quadratic (or equivalently that the sampling distribution of the estimated parameters is normal).

```
> summary(m0)
```

Maximum likelihood estimation

```
Call:
```

```
mle2(minuslog1 = mtmp, start = list(prob = 0.2, theta = 9), data = list(size = 50))
```

Coefficients:

```
Estimate Std. Error z value Pr(z)
prob 0.1030974 0.0031626 32.599 < 2.2e-16 ***
theta 10.0758090 0.6213010 16.217 < 2.2e-16 ***
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

-2 log L: 5446.995

Construct the likelihood profile (you can apply confint directly to m0, but if you're going to work with the likelihood profile [e.g. plotting, or looking for confidence intervals at several different α values] then it is more efficient to compute the profile once):

```
> p0 <- profile(m0)
```

Compare the confidence interval estimates based on inverting a spline fit to the profile (the default); based on the quadratic approximation at the maximum likelihood estimate; and based on root-finding to find the exact point where the profile crosses the critical level.

> confint(p0)

```
2.5 % 97.5 % prob 0.09709228 0.1095103 theta 8.91708221 11.3559589
```

> confint(m0,method="quad")

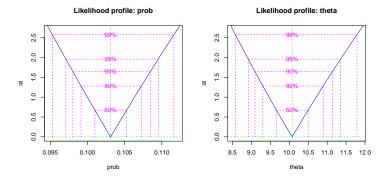
2.5 % 97.5 % prob 0.09689876 0.1092961 theta 8.85808147 11.2935366

> confint(m0,method="uniroot")

2.5 % 97.5 % prob 0.09709185 0.1095099 theta 8.91691020 11.3559746

All three types of confidence limits are similar. Plot the profiles:

- > par(mfrow=c(1,2))
- > plot(p0,plot.confstr=TRUE)



By default, the plot method for likelihood profiles displays the square root of the the deviance difference (twice the difference in negative log-likelihood from the best fit), so it will be V-shaped for cases where the quadratic approximation works well (as in this case). (For a better visual estimate of whether the profile is quadratic, use the absVal=FALSE option to the plot method.)

You can also request confidence intervals calculated using uniroot, which may be more exact when the profile is not smooth enough to be modeled accurately by a spline. However, this method is also more sensitive to numeric problems.

Instead of defining an explicit function for minuslog1, we can also use the formula interface. The formula interface assumes that the density function given (1) has x as its first argument (if the distribution is multivariate, then x should be a matrix of observations) and (2) has a log argument that will return the log-probability or log-probability density if log=TRUE. Some of the extended functionality (prediction etc.) depends on the existence of an s- variant function for the distribution that returns (at least) the mean and median as a function of the parameters (currently defined: snorm, sbinom, sbeta, snbinom, spois).

Note that you must specify the data via the data argument when using the formula interface. This may be slightly more unwieldy than just pulling the data from your workspace when you are doing simple things, but in the long run it makes tasks like predicting new responses much simpler.

It's convenient to use the formula interface to try out likelihood estimation on the transformed parameters:

In this case the answers from uniroot and spline (default) methods barely differ.

1.2 Real data (Orobanche, Crowder (1978))

Data as incorporated in the aod package:

```
> library(aod)
Package aod, version 1.2
> data(orob1)
```

Now construct a negative log-likelihood function that differentiates among groups:

```
> ML1 <- function(prob1,prob2,prob3,theta,x) {
   prob <- c(prob1,prob2,prob3)[as.numeric(x$dilution)]
   size <- x$n
   -sum(dbetabinom(x$y,prob,size,theta,log=TRUE))
}</pre>
```

Results from Crowder (1978):

| model | prob1 | prob2 | prob3 | theta | sd.prob1 | sd.prob2 | sd.prob3 | NLL |
|-------------|-------|-------|-------|--------|----------|----------|----------|---------|
| prop diffs | 0.132 | 0.871 | 0.839 | 78.424 | 0.027 | 0.028 | 0.032 | -34.991 |
| full model | | | | | | | | -34.829 |
| homog model | | | | | | | | -56.258 |

Call:

```
mle2(minuslogl = ML1, start = list(prob1 = 0.5, prob2 = 0.5,
    prob3 = 0.5, theta = 1), data = list(x = orob1))
```

Coefficients:

```
prob1 prob2 prob3 theta
0.1318187 0.8706259 0.8382504 73.7968323
```

Log-likelihood: -34.99

Warning: optimization did not converge (code 1:)

Or: The result warns us that the optimization has not converged; we also don't match Crowder's results for θ exactly. We can fix this by setting parscale appropriately.

Call:

Coefficients:

```
prob1 prob2 prob3 theta 0.1322123 0.8708913 0.8393195 78.4227905
```

Log-likelihood: -34.99

Calculate likelihood profile (restrict the upper limit of θ , simply because it will make the picture below a little bit nicer):

```
> p2 <- profile(m2,prof.upper=c(Inf,Inf,Inf,theta=2000))</pre>
```

Get the curvature-based parameter standard deviations (which Crowder used rather than computing likelihood profiles):

```
> round(sqrt(diag(vcov(m2))),3)

prob1 prob2 prob3 theta
0.028 0.029 0.032 74.223

We are slightly off Crowder's numbers — rounding error?

Crowder also defines a variance (overdispersion) parameter \sigma^2 = 1/(1+\theta).

> sqrt(1/(1+coef(m2)["theta"]))

theta
0.1122089
```

Using the delta method (via the deltavar function in the emdbook package) to approximate the standard deviation of σ :

[1] 0.0524311

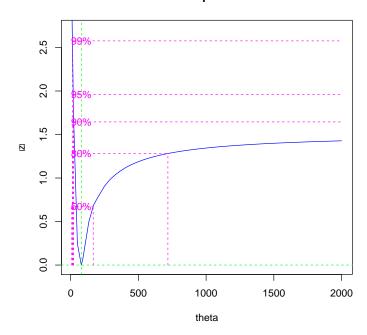
Another way to fit in terms of σ rather than θ is to compute $\theta = 1/\sigma^2 - 1$ on the fly in a formula:

As might be expected since the standard deviation of σ is large, the quadratic approximation is poor:

Plot the profile:

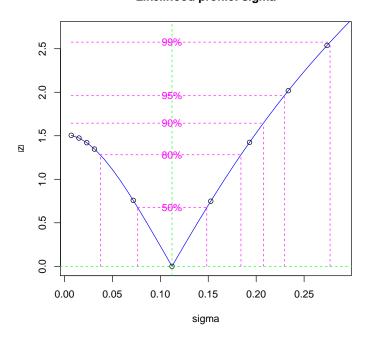
> plot(p2,which="theta",plot.confstr=TRUE)

Likelihood profile: theta



What does the profile for σ look like?

Likelihood profile: sigma



Now fit a homogeneous model:

The log-likelihood matches Crowder's result:

```
> logLik(m0)
```

```
'log Lik.' -56.25774 (df=2)
```

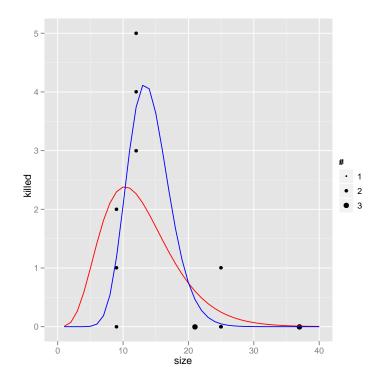
It's easier to use the formula interface to specify all three of the models fitted by Crowder (homogeneous, probabilities differing by group, probabilities and overdispersion differing by group):

```
parameters=list(prob~dilution,theta~1),
             data=orob1,
             start=list(prob=0.5, theta=78.424))
> m3f <- mle2(y~dbetabinom(prob,size=n,theta),</pre>
             parameters=list(prob~dilution,theta~dilution),
             data=orob1,
             start=list(prob=0.5,theta=78.424))
   anova runs a likelihood ratio test on nested models:
> anova(m0f, m2f, m3f)
Likelihood Ratio Tests
Model 1: mOf, y~dbetabinom(prob,size=n,theta): prob~1, theta~1
Model 2: m2f, y~dbetabinom(prob,size=n,theta): prob~dilution, theta~1
Model 3: m3f, y~dbetabinom(prob,size=n,theta): prob~dilution,
          theta~dilution
                  Chisq Df Pr(>Chisq)
 Tot Df Deviance
       2 112.515
1
       4 69.981 42.5341 2 5.805e-10 ***
3
       6 69.981 0.0008 2
                                 0.9996
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
   The various ICtab commands produce tables of information criteria, option-
ally sorted and with model weights.
> AICtab(mOf, m2f, m3f, weights=TRUE, delta=TRUE, sort=TRUE)
    dAIC df weight
m2f 0.0 4 0.881
m3f 4.0 6 0.119
mOf 38.5 2 <0.001
> BICtab(mOf,m2f,m3f,delta=TRUE,nobs=nrow(orob1),sort=TRUE,weights=TRUE)
    dBIC df weight
m2f 0.0 4 0.9412
m3f 5.5 6 0.0588
mOf 37.0 2 <0.001
> AICctab(mOf, m2f, m3f, delta=TRUE, nobs=nrow(orob1), sort=TRUE, weights=TRUE)
    dAICc df weight
m2f 0.0 4 0.99222
m3f 9.7 6 0.00778
mOf 35.8 2 < 0.001
```

2 Example: reed frog size predation

```
Data from an experiment by Vonesh (Vonesh and Bolker, 2005)
```

```
> frogdat <- data.frame(</pre>
   size=rep(c(9,12,21,25,37),each=3),
   killed=c(0,2,1,3,4,5,rep(0,4),1,rep(0,4)))
> frogdat$initial <- rep(10,nrow(frogdat))</pre>
> library(ggplot2)
> gg1 <- ggplot(frogdat,aes(x=size,y=killed))+geom_point()+
       stat_sum(aes(size=factor(..n..)))+
       labs(size="#")+scale_x_continuous(limits=c(0,40))
> m3 <- mle2(killed~dbinom(prob=c*(size/d)^g*exp(1-size/d),</pre>
   size=initial),data=frogdat,start=list(c=0.5,d=5,g=1))
> pdat <- data.frame(size=1:40,initial=rep(10,40))</pre>
> pdat1 <- data.frame(pdat,killed=predict(m3,newdata=pdat))</pre>
> m4 <- mle2(killed~dbinom(prob=c*((size/d)*exp(1-size/d))^g,
   size=initial),data=frogdat,start=list(c=0.5,d=5,g=1))
> pdat2 <- data.frame(pdat,killed=predict(m4,newdata=pdat))</pre>
> print(gg1 + geom_line(data=pdat1,colour="red")+
       geom_line(data=pdat2,colour="blue"))
```



> coef(m4)

0.4138847 13.3517574 18.2511264

> prof4 <- profile(m4)</pre>

Three different ways to draw the profile:

(1) Built-in method (base graphics):

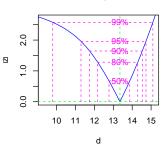
> print(plot(prof4))

NULL

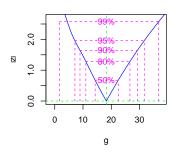
Likelihood profile: c

2.0 1.0 0.2 0.4 0.6 0.8 С

Likelihood profile: d



Likelihood profile: g



(2) Using xyplot from the lattice package:

```
> prof4_df <- as.data.frame(prof4)</pre>
```

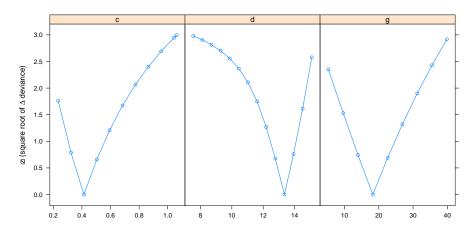
- > library(lattice)
- > print(xyplot(abs(z)~focal|param,data=prof4_df, subset=abs(z)<3,

type="b",

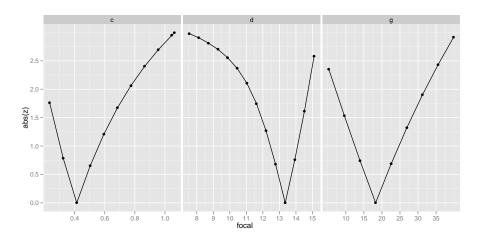
xlab="",

ylab=expression(paste(abs(z),

" (square root of ",Delta, " deviance)")), scale=list(x=list(relation="free")), layout=c(3,1))



(3) Using ggplot from the ggplot2 package:



Additions/enhancements/differences from stats4::mle

- \bullet anova method
- warnings on convergence failure
- more robust to non-positive-definite Hessian; can also specify skip.hessian to skip Hessian computation when it is problematic
- $\bullet\,$ when profiling fails because better value is found, report new values

- can take named vectors as well as lists as starting parameter vectors
- added AICc, BIC definitions, ICtab functions
- added "uniroot" and "quad" options to confint
- more options for colors and line types etc etc. The old arguments are:

```
> function (x, levels, conf = c(99, 95, 90, 80, 50)/100, nseg = 50, absVal = TRUE, ...) {}
```

The new one is:

which selects (by character vector or numbers) which parameters to plot: nseg does nothing (even in the old version); plot.confstr turns on the labels for the confidence levels; confstr gives the labels; add specifies whether to add the profile to an existing plot; col and lty options specify the colors and line types for horizontal and vertical lines marking the minimum and confidence vals and the profile curve; xlabs gives a vector of x labels; ylab gives the y label; show.points specifies whether to show the raw points computed.

- mle.options()
- data argument
- handling of names in argument lists
- can use alternative optimizers (nlminb, nlm, constrOptim, optimx, optimize)
- uses code from numDeriv package to compute Hessians rather than built-in optimizer code
- by default, uses MASS::ginv (generalized inverse) rather than solve to invert Hessian (more robust to positive-semidefinite Hessians...)
- can use vecpar=TRUE (and parnames()) to use objective functions with parameters specified as vectors (for compatibility with optim etc.)

3 Newer stuff

To do:

- use predict, simulate etc. to demonstrate different parametric bootstrap approaches to confidence and prediction intervals
 - use predict to get means and standard deviations, use delta method?
 - use vcov, assuming quadratic profiles, with predict(...,newparams=...)
 - prediction intervals assuming no parameter uncertainty with simulate
 - both together ...

4 Technical details

4.1 Profiling and confidence intervals

This section describes the algorithm for constructing profiles and confidence intervals, which is not otherwise documented anywhere except in the code. * indicates changes from the version in stats4:::mle

4.1.1 Estimating standard error

In order to construct the profile for a particular parameter, one needs an initial estimate of the scale over which to vary that parameter. The estimated standard error of the parameter based on the estimated curvature of the likelihood surface at the MLE is a good guess.

- if std.err is missing, extract the standard error from the summary coefficient table (ultimately computed from sqrt(diag(inverse Hessian)) of the fit)
- * a user-set value of std.err overrides this behavior unless the value is specified as NA (in which case the estimate from the previous step is used)
- * if the standard error value is still NA (i.e. the user did not specify it and the value estimated from the Hessian is missing or NA) use sqrt(1/diag(hessian)). This represents a (fairly feeble) attempt to come up with a plausible number when the Hessian is not positive definite but still has positive diagonal entries
- if all else fails, stop and * print an error message that encourages the user to specify the values with std.err

There may be further tricks that would help guess the appropriate scale: for example, one could guess on the basis of a comparison between the parameter values and negative log-likelihoods at the starting and ending points of the fits.

On the other hand, (a) this would take some effort and still be subject to failure for sufficiently pathological fits and (b) there is some value to forcing the user to take explicit, manual steps to remedy such problems, as they may be signs of poorly defined or buggy log-likelihood functions.

4.1.2 Profiling

Profiling is done on the basis of a constructed function that minimizes the negative log-likelihood for a fixed value of the focal parameter and returns the signed square-root of the deviance difference from the minimum (denoted by z). At the MLE z=0 by definition; it should never be <0 unless something has gone wrong with the original fit. The LRT significance cutoffs for z are equal to the usual two-tailed normal distribution cutoffs (e.g. $\pm \approx 1.96$ for 95% confidence regions).

In each direction (decreasing and increasing from the MLE for the focal parameter):

- fix the focal parameter
- adjust control parameters etc. accordingly (e.g. remove the entry for the focal parameter so that the remaining control parameters match the non-fixed parameters)
- controls on the profiling (which can be set manually, but for which there is not much guidance in the documentation):
 - zmax Maximum z to aim for. (Default: sqrt(qchisq(1-alpha/2, p))) The default maximum α (type I error) is 0.01. I don't understand this criterion. It seems to expand the size of the univariate profile to match a cutoff for the multivariate confidence region of the model. The χ^2 cutoff for deviance to get the $(1-\alpha)$ multivariate confidence region (i.e., on all p of the parameters) would be qchisq(1-alpha,p) representing a one-tailed test on the deviance. Taking the square root makes sense, since we are working with the square root of the deviance, but I don't understand (1) why we are expanding the region to allow for the multivariate confidence region (since we are computing univariate profiles) [you could at least argue that this is conservative, making the region a little bigger than it needs to be]; (2) why we are using $1-\alpha/2$ rather than $1-\alpha$.
 - del Step size (scaled by standard error) (Default: zmax/5.) This seems reasonable, but I don't know where it comes from.
 - maxsteps Maximum number of profiling steps to try in each direction.
 (Default: 100)
- While step<maxsteps and abs(z) < zmax, set the value of the focal parameter to its MLE + sgn*step*del*std.err where sgn represents the direction, step is the current (integer) step, and del and std.err are the

step size scaling factor and standard error estimate discussed above (i.e. take steps of size (del*std.err) in the appropriate direction); evaluate z

- Stop the profiling:
 - if z doesn't change from the previous step (stop_flat)
 - * stop if z is less than tol.newmin (default: 0.001) units better than the MLE fit, i.e. z < -tol.newmin (if -tol.newmin < z < 0, set z to zero) (newpars_found)
 - if z is NA (stop_na) (for greater robustness, should we try to keep
 going anyway?)
 - if z is beyond zmax (i.e., we have reached our goal: stop_cutoff)
 - if step==maxsteps
 - if the focal parameter has hit its upper/lower bound (stop_bound)
- if we have hit the maximum number of steps but not reached the cutoff (stop_maxstep but not stop_cutoff), "try a bit harder": go almost one more del*std.err unit out (in intervals of 0.2, 0.4, 0.6, 0.8, 0.9) (also seems reasonable but don't know where it comes from)
- * if we violated the boundary but did not reach the cutoff (!stop_cutoff && stop_bound), evaluate z at the boundary
- if we got to the cutoff in < 5 steps, try smaller steps: start at step=0.5 and proceed to mxstep-0.5 in unit increments (rather than the original scale which went from 0 to mxstep). (Again, it seems reasonable, but I don't know what the original justification was ...)

4.1.3 Confidence intervals

We are looking for the values where z (signed square root deviance difference) is equal to the usual two-tailed normal distribution cutoffs for a specified α level, e.g. $z=\pm 1.96$ for 95% confidence intervals (this is equivalent to a one-tailed test on the deviance difference with the cutoff value for χ_1^2).

- If necessary, construct the profile
- * If the profile of the signed square root is non-monotonic, warn the user and revert to linear approximation on the profiled points to find the cutoffs:
- Otherwise, build an interpolation spline of z (signed square root deviance difference) based on profiled points (the default is $n=3\times L$ where L is the length of the original vector). Then use linear approximation on the y(z) and x (focal parameter value) of the spline to find the cutoffs (Why construct a spline and then interpolate linearly? Why not use backSpline as in the profile plotting code?)

It is also possible to use method="quad" (this is obsolete, should be replaced by documentation pointing to confint.default) and method="uniroot" (undocumented for now; rather than approximating from the profile, try to use uniroot with calls to the negative log-likelihood function to identify the confidence intervals as precisely and robustly as possible (should be more accurate, but slower — must also be computed for each specified α level separately).

4.1.4 Profile plotting

Plot the signed (or unsigned) square root deviance difference, and $(1 - \alpha)$ confidence regions/critical values designated by **conf** (default: $\{0.99, 0.95, 0.9, 0.8, 0.5\}$).

- * If the (signed) profile is non-monotonic, simply plot computed points with type="l" (i.e., with the default linear interpolation)
- Construct the interpolation spline (using splines:::interpSpline rather than spline as in the confidence interval method (why this difference?)
- attempt to construct the inverse of the interpolation spline (using back-Spline)
- * if this fails warn the user (assume this was due to non-monotonicity) and try to use uniroot and predict to find cutoff values
- otherwise, use the inverse spline to find cutoff values

Why is there machinery in the plotting code to find confidence intervals? Shouldn't this call confint, for consistency/fewer points of failure?

Bugs, wishes, to do

- WISH: further methods and arguments: subset, predict, resid: sim?
- WISH: extend ICtab to allow DIC as well?
- minor **WISH**: better methods for extracting **nobs** information when possible (e.g. with formula interface)
- WISH: better documentation, especially for S4 methods
- WISH: variable-length chunks in argument list
- **WISH**: limited automatic differentiation (add capability for common distributions)

References

Crowder, M. J. (1978). Beta-binomial Anova for proportions. *Applied Statistics* 27, 34–37.

Vonesh, J. R. and B. M. Bolker (2005). Compensatory larval responses shift tradeoffs associated with predator-induced hatching plasticity. Ecology~86 (6), 1580–1591.