Maximum likelihood estimation and analysis with the `bbmle` package

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Contents

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 slightly 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 `aod` and `vgam` (on CRAN), `gnlr` and `gnlr3` in Jim Lindsey's `gnlm` package (`http://popgen.unimaas.nl/~jlindsey/rcode.html`).

1 Example

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:

```
> mtmp <- function(prob,size,theta) {
   -sum(dbetabinom(x1,prob,size,theta,log=TRUE))
 }
```

Fit the model — use `data` to pass the `size` parameter (since it wasn't hard-coded in the `mtmp` function):

```
> (m0 <- mle2(mtmp,start=list(prob=0.2,theta=9),data=list(size=50)))

Call:
mle2(minuslogl = mtmp, start = list(prob = 0.2, theta = 9), data = list(size = 50))

Coefficients:
      prob      theta
 0.1030974 10.0758090

Log-likelihood: -2723.5
```

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 of normality.

```
> summary(m0)

Maximum likelihood estimation

Call:
mle2(minuslogl = mtmp, start = list(prob = 0.2, theta = 9), data = list(size = 50))

Coefficients:
        Estimate Std. Error z value     Pr(z)
prob   0.1030974  0.0031624  32.601 < 2.2e-16 ***
theta 10.0758090  0.6212681  16.218 < 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)
```

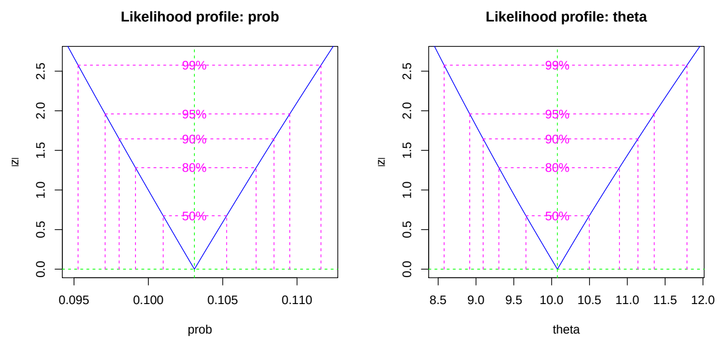
Compare the confidence interval estimates based on inverting a spline fit to the profile (the default); based on the quadratic approximation at the maximum likelihood estimate; and based on root-finding to find the exact point where the profile crosses the critical level.

```
> confint(p0)

           2.5 %     97.5 %
prob  0.09709228  0.1095103
theta 8.91708238 11.3559585

> confint(m0,method="quad")

           2.5 %     97.5 %
prob  0.09689924  0.1092956
theta 8.85814593 11.2934721

> 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 (twice the difference in negative log-likelihood), 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 `minuslogl`, 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`.

```
> m0f <- mle2(x1~dbetabinom(prob,size=50,theta),
             start=list(prob=0.2,theta=9),data=data.frame(x1))
```

Note that you must specify the data via the `data` argument when using the formula interface; this is sometimes 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:

```
> m0cf <- mle2(x1~dbetabinom(prob=plogis(lprob),size=50,theta=exp(ltheta)),
             start=list(lprob=0,ltheta=2),data=data.frame(x1))
> confint(m0cf,method="uniroot")

           2.5 %    97.5 %
lprob  -2.229963 -2.095757
ltheta  2.187950  2.429744
```

```
> confint(m0cf,method="spline")
```

```
          2.5 %    97.5 %
lprob  -2.229963 -2.095756
ltheta  2.187948  2.429742
```

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))
 }
```

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

```
> (m1 <- mle2(ML1,start=list(prob1=0.5,prob2=0.5,prob3=0.5,theta=1),
     data=list(x=orob1)))
```

```
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
 0.1318283  0.8706206  0.8382693 73.6993151

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.

```
> (m2 <- mle2(ML1,start=as.list(coef(m1)),
           control=list(parscale=coef(m1)),
           data=list(x=orob1)))

0.1322123 0.8708914 0.8393195 78.42279

Call:
mle2(minuslogl = ML1, start = as.list(coef(m1)), data = list(x = orob1),
    control = list(parscale = coef(m1)))

Coefficients:
     prob1      prob2      prob3      theta
 0.1322123  0.8708914  0.8393195 78.4227872

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))
```

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 74.213
```

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:

```
> sqrt(deltavar(sqrt(1/(1+theta)),meanval=coef(m2)["theta"],
          vars="theta",Sigma=vcov(m2)[4,4]))

[1] 0.0524241
```

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:

```
> m2b <- mle2(y~dbetabinom(prob,size=n,theta=1/sigma^2-1),
             data=orob1,
             parameters=list(prob~dilution,sigma~1),
             start=list(prob=0.5,sigma=0.1))
> round(sqrt(diag(vcov(m2b))),3)["sigma"]
```

```
sigma
0.052
```

```
> p2b <- profile(m2b,prof.lower=c(-Inf,-Inf,-Inf,0))
```

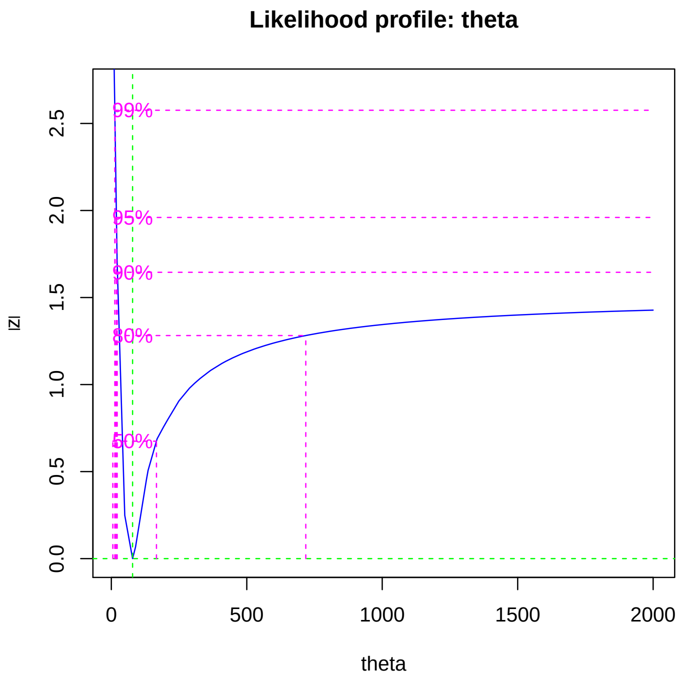
As might be expected since the standard deviation of σ is large, the quadratic approximation is poor:

```
> r1 <- rbind(confint(p2)["theta",],
             confint(m2,method="quad")["theta",])
> rownames(r1) <- c("spline","quad")
> r1
```

```
            2.5 %   97.5 %
spline  19.67247        NA
quad   -67.03157 223.8771
```

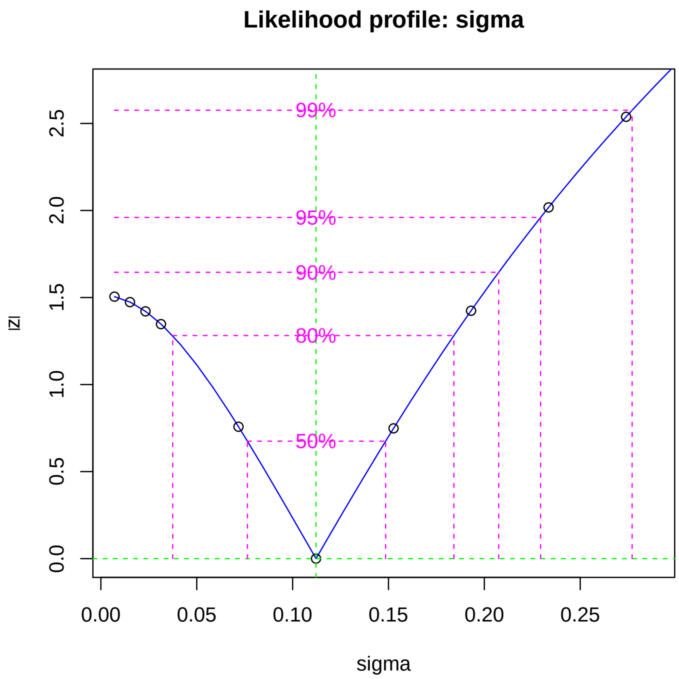
Plot the profile:

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



What does the profile for σ look like?

```
> plot(p2b,which="sigma",plot.confstr=TRUE,
      show.points=TRUE)
```



Now fit a homogeneous model:

```
> ml0 <- function(prob,theta,x) {
   size <- x$n
   -sum(dbetabinom(x$y,prob,size,theta,log=TRUE))
 }
> m0 <- mle2(ml0,start=list(prob=0.5,theta=100),
           data=list(x=orob1))
```

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):

```
> m0f <- mle2(y~dbetabinom(prob,size=n,theta),
             parameters=list(prob~1,theta~1),
             data=orob1,
             start=list(prob=0.5,theta=100))
> m2f <- mle2(y~dbetabinom(prob,size=n,theta),
```

```
             parameters=list(prob~dilution,theta~1),
             data=orob1,
             start=list(prob=0.5,theta=78.424))
> m3f <- mle2(y~dbetabinom(prob,size=n,theta),
             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: m0f, 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
  Tot Df Deviance   Chisq Df Pr(>Chisq)
1      2  112.515
2      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, optionally sorted and with model weights.

```
> AICtab(m0f,m2f,m3f,weights=TRUE,delta=TRUE,sort=TRUE)

    dAIC df weight
m2f  0.0 4  0.881
m3f  4.0 6  0.119
m0f 38.5 2  <0.001

> BICtab(m0f,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
m0f 37.0 2  <0.001

> AICctab(m0f,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
m0f 35.8  2  < 0.001
```

Additions/enhancements/differences from `stats4::mle`

- `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
- 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:

  ```
  > function (x, levels, which=1:p, conf = c(99, 95, 90, 80, 50)/100, nseg = 50,
              plot.confstr = FALSE, confstr = NULL, absVal = TRUE, add = FALSE,
              col.minval="green", lty.minval=2,
              col.conf="magenta", lty.conf=2,
              col.prof="blue", lty.prof=1,
              xlabs=nm, ylab="score",
              show.points=FALSE,
              main, xlim, ylim, ...) {}
  ```

  `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`, `constrOptim`)

2 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 ...

3 Example

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

```
> frogdat <- data.frame(
  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))
```

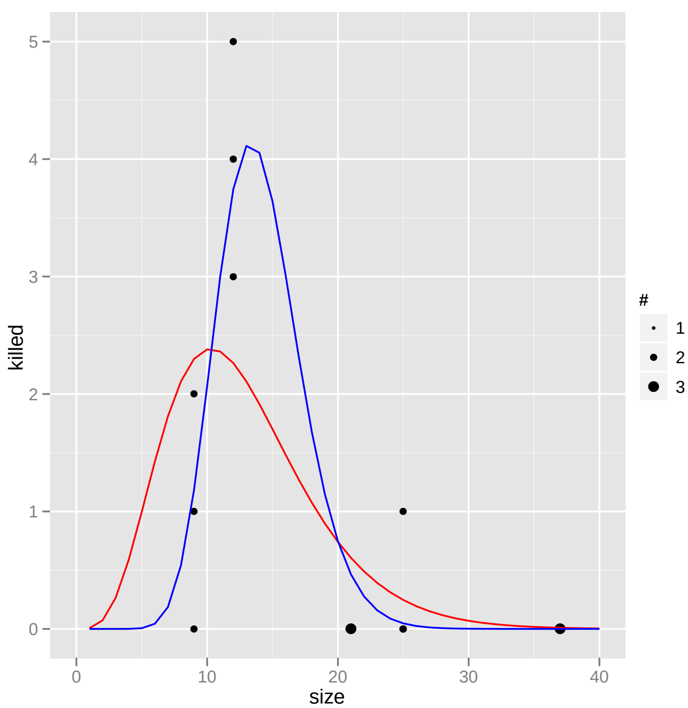
```
> library(ggplot2)
```

```
> 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),
  size=initial),data=frogdat,start=list(c=0.5,d=5,g=1))
> pdat <- data.frame(size=1:40,initial=rep(10,40))
> pdat1 <- data.frame(pdat,killed=predict(m3,newdata=pdat))
```

```
> 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))
```

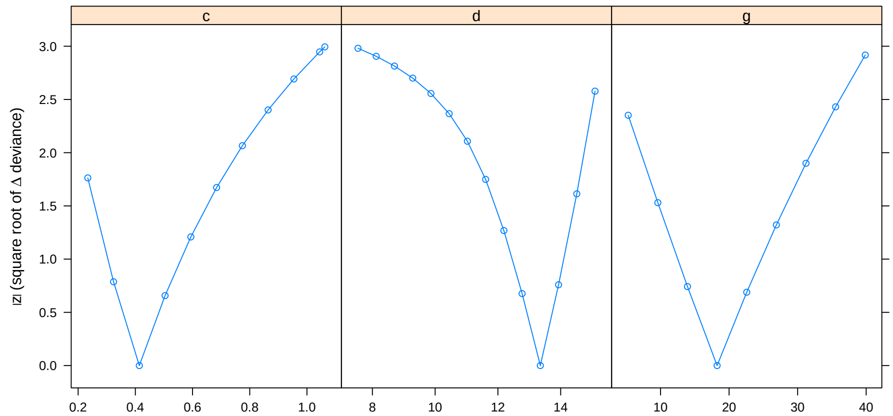
```
> print(gg1 + geom_line(data=pdat1,colour="red")+geom_line(data=pdat2,colour="blue"))
```



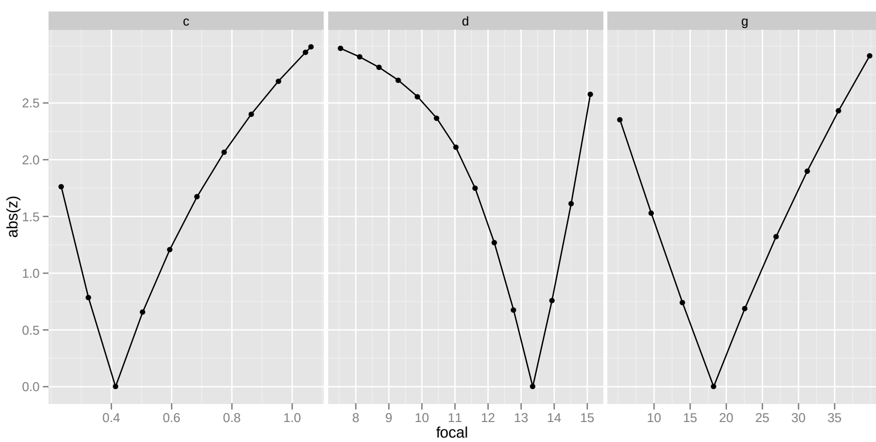

```
> coef(m4)

         c          d          g
 0.4138847 13.3517574 18.2511264

> prof4 <- profile(m4)
```

Three different ways to draw the profile:

```
> print(plot(prof4))

NULL

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




```
> print(ggplot(subset(prof4_df,abs(z)<3),
         aes(x=focal,y=abs(z)))+geom_line()+
       geom_point()+
       facet_grid(~param,scale="free_x"))
```



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.