Maximum likelihood estimation and analysis with the `bbmle` package

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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.
- `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 [1] (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.

Implement beta-binomial distribution (density and random-deviate function — these functions are also available in the `emdbook` package, and in Jim Lindsey's `rmutil` package).

```
> dbetabinom <- function(x, mu, size, theta, log = FALSE) {
+     v <- lchoose(size, x) - lbeta(theta * (1 - mu), theta *
+         mu) + lbeta(size - x + theta * (1 - mu), x +
+         theta * mu)
+     if (log)
+         v
+     else exp(v)
+ }
> rbetabinom <- function(n, mu, size, theta) {
+     a <- theta * mu
+     b <- theta * (1 - mu)
+     rbinom(n, size = size, prob = rbeta(n, a, b))
+ }
```

Generate random deviates from a random beta-binomial:

```
> set.seed(1001)
> x1 = rbetabinom(n = 1000, mu = 0.1, size = 50, theta = 10)
```

Load the package:

```
> library(bbmle)
```

Construct a simple negative log-likelihood function:

```
> mtmp <- function(mu, size, theta) {
+     -sum(dbetabinom(x1, mu, 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(mu = 0.2, theta = 9), data = list(size = 50))
> m0

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

Coefficients:
        mu      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(mu = 0.2, theta = 9), data = list(size = 50))

Coefficients:
        Estimate Std. Error z value     Pr(z)    
mu     0.1030974  0.0031624  32.601 < 2.2e-16 ***
theta 10.0758090  0.6213189  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)
```

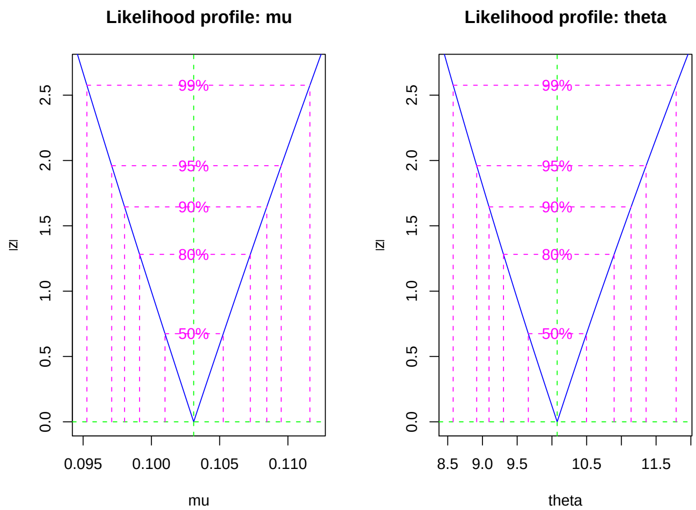
Compare the confidence interval estimates based on inverting a spline fit to the profile (the default); based on the quadratic approximation at the maximum likelihood estimate; and based on root-finding to find the exact point where the profile crosses the critical level.

```
> confint(p0)

           2.5 %     97.5 %
mu    0.09709228  0.1095103
theta 8.91708211 11.3559591

> confint(m0, method = "quad")

           2.5 %     97.5 %
mu    0.09689929  0.1092955
theta 8.85804640 11.2935716

> confint(m0, method = "uniroot")

           2.5 %     97.5 %
mu    0.09709185  0.1095099
theta 8.91691019 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 `absVal=FALSE`.)

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(mu, size = 50, theta), start = list(mu = 0.2,
+     theta = 9))
```

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

```
> m0cf <- mle2(x1 ~ dbetabinom(mu = plogis(lmu), size = 50,
+     theta = exp(ltheta)), start = list(lmu = 0, ltheta = 2))
> confint(m0cf, method = "uniroot")
```

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

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

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

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

1.2 Using real data

Get data from Crowder 1978 [1], as incorporated in the `aod` package:

```
> library(aod)
```

```
Package aod, version 1.1-22
```

```
> data(orob1)
```

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

```
> ML1 <- function(mu1, mu2, mu3, theta, x) {
+     mu <- c(mu1, mu2, mu3)[as.numeric(x$dilution)]
+     size <- x$n
+     -sum(dbetabinom(x$y, mu, size, theta, log = TRUE))
+ }
```

Results from [1]:

model	mu1	mu2	mu3	theta	sd.mu1	sd.mu2	sd.mu3	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(mu1 = 0.5, mu2 = 0.5, mu3 = 0.5,
+     theta = 1), data = list(x = orob1))
> m1
```

```
Call:
mle2(minuslogl = ML1, start = list(mu1 = 0.5, mu2 = 0.5, mu3 = 0.5,
    theta = 1), data = list(x = orob1))

Coefficients:
```

```
       mu1        mu2        mu3      theta
 0.1318287  0.8706204  0.8382700 73.6958477

Log-likelihood: -34.99

Warning: optimization did not converge (code 1)
```

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))
```

```
> m2
```

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

Coefficients:
       mu1        mu2        mu3      theta
 0.1322123  0.8708914  0.8393195 78.4227872

Log-likelihood: -34.99
```

Calculate likelihood profile:

```
> p2 <- profile(m2)
```

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

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

```
   mu1    mu2    mu3  theta
 0.028  0.029  0.032 74.238
```

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 to get the standard deviation of σ:

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

```
[1] 0.05244163
```

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

```
sigma
0.052
```

```
> p2b <- profile(m2b)
```

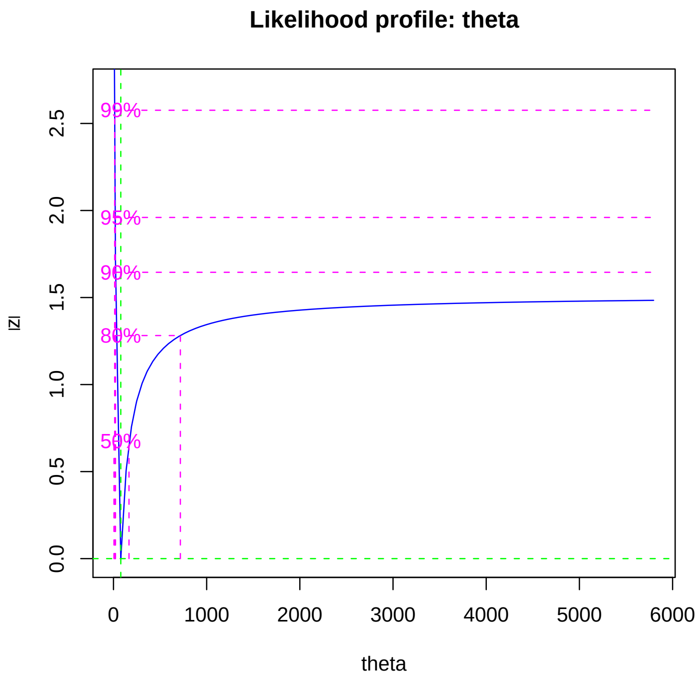
As might be expected since the standard deviation of σ is large, the quadratic approximation is poor:

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

```
           2.5 %   97.5 %
spline  19.81826       NA
quad   -67.08021 223.9258
```

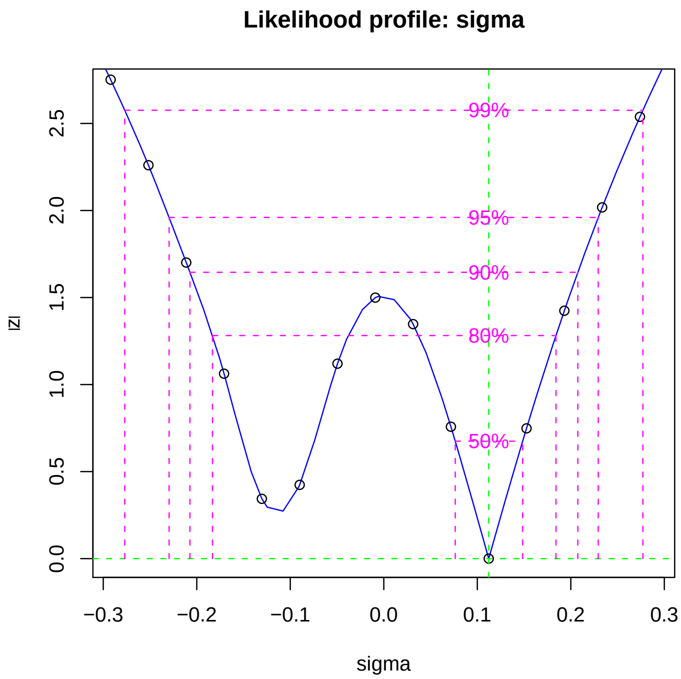
Plot the profile:

```
> 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(mu, theta, x) {
+     size <- x$n
+     -sum(dbetabinom(x$y, mu, size, theta, log = TRUE))
+ }
> m0 <- mle2(ml0, start = list(mu = 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(mu, size = n, theta), parameters = list(mu ~
+     1, theta ~ 1), data = orob1, start = list(mu = 0.5,
+     theta = 100))
> m2f <- mle2(y ~ dbetabinom(mu, size = n, theta), parameters = list(mu ~
+     dilution, theta ~ 1), data = orob1, start = list(mu = 0.5,
```

```
+     theta = 78.424))
> m3f <- mle2(y ~ dbetabinom(mu, size = n, theta), parameters = list(mu ~
+     dilution, theta ~ dilution), data = orob1, start = list(mu = 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(mu,size=n,theta): mu~1, theta~1
Model 2: m2f, y~dbetabinom(mu,size=n,theta): mu~dilution, theta~1
Model 3: m3f, y~dbetabinom(mu,size=n,theta): mu~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)

    AIC   df dAIC  weight
m2f  78.0 4    0.0 0.881
m3f  82.0 6    4.0 0.119
m0f 116.5 2   38.5 <0.001

> BICtab(m0f, m2f, m3f, delta = TRUE, nobs = nrow(orob1),
+     sort = TRUE, weights = TRUE)

    BIC   df dBIC  weight
m2f  81.1 4    0.0 0.941
m3f  86.6 6    5.5 0.059
m0f 118.1 2   37.0 <0.001

> AICctab(m0f, m2f, m3f, delta = TRUE, nobs = nrow(orob1),
+     sort = TRUE, weights = TRUE)

    AICc  df dAICc weight
m2f  81.6 4    0.0 0.992
m3f  91.3 6    9.7 0.008
m0f 117.4 2   35.8 <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`)

Bugs, wishes, to do

- **BUG**: `mle2` fits that are obtained within a function can't be used for subsequent profiles etc. (environment issue)
- **WISH**: `subset` and `predict`
- 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

[1] Martin J. Crowder. Beta-binomial Anova for proportions. *Applied Statistics*, 27(1):34–37, 1978.