Estimating Non-Linear Models with brms

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2019-05-22

Introduction

This vignette provides an introduction on how to fit non-linear multilevel models with **brms**. Non-linear models are incredibly flexible and powerful, but require much more care with respect to model specification and priors than typical generalized linear models. Ignoring group-level effects for the moment, the predictor term η_n of a generalized linear model for observation n can be written as follows:

$$\eta_n = \sum_{i=1}^{K} b_i x_{ni}$$

where b_i is the regression coefficient of predictor i and x_{ni} is the data of predictor i for observation n. This also compromises interaction terms and various other data transformations. However, the structure of η_n is always linear in the sense that the regression coefficients b_i are multiplied by some predictor values and then summed up. This implies that the hypothetical predictor term

$$\eta_n = b_1 \exp(b_2 x_n)$$

would *not* be a *linear* predictor anymore and we could not fit it using classical techniques of generalized linear models. We thus need a more general model class, which we will call *non-linear* models. Note that the term 'non-linear' does not say anything about the assumed distribution of the response variable. In particular it does not mean 'not normally distributed' as we can apply non-linear predictor terms to all kinds of response distributions (for more details on response distributions available in **brms** see `vignette("brms_families")`).

A Simple Non-Linear Model

We begin with a simple example using simulated data.

```r
b <- c(2, 0.75)
x <- rnorm(100)
```

```
y <- rnorm(100, mean = b[1] * exp(b[2] * x))
dat1 <- data.frame(x, y)
```

As stated above, we cannot use a generalized linear model to estimate b so we go ahead an specify a non-linear model.

```
prior1 <- prior(normal(1, 2), nlpar = "b1") +
  prior(normal(0, 2), nlpar = "b2")
fit1 <- brm(bf(y ~ b1 * exp(b2 * x), b1 + b2 ~ 1, nl = TRUE),
            data = dat1, prior = prior1)
```

When looking at the above code, the first thing that becomes obvious is that we changed the `formula` syntax to display the non-linear formula including predictors (i.e., `x`) and parameters (i.e., `b1` and `b2`) wrapped in a call to `bf`. This stands in contrast to classical **R** formulas, where only predictors are given and parameters are implicit. The argument `b1 + b2 ~ 1` serves two purposes. First, it provides information, which variables in `formula` are parameters, and second, it specifies the linear predictor terms for each parameter. In fact, we should think of non-linear parameters as placeholders for linear predictor terms rather than as parameters themselves (see also the following examples). In the present case, we have no further variables to predict `b1` and `b2` and thus we just fit intercepts that represent our estimates of b_1 and b_2 in the model equation above. The formula `b1 + b2 ~ 1` is a short form of `b1 ~ 1, b2 ~ 1` that can be used if multiple non-linear parameters share the same formula. Setting `nl = TRUE` tells **brms** that the formula should be treated as non-linear.

In contrast to generalized linear models, priors on population-level parameters (i.e., 'fixed effects') are often mandatory to identify a non-linear model. Thus, **brms** requires the user to explicitely specify these priors. In the present example, we used a `normal(1, 2)` prior on (the population-level intercept of) `b1`, while we used a `normal(0, 2)` prior on (the population-level intercept of) `b2`. Setting priors is a non-trivial task in all kinds of models, especially in non-linear models, so you should always invest some time to think of appropriate priors. Quite often, you may be forced to change your priors after fitting a non-linear model for the first time, when you observe different MCMC chains converging to different posterior regions. This is a clear sign of an idenfication problem and one solution is to set stronger (i.e., more narrow) priors.

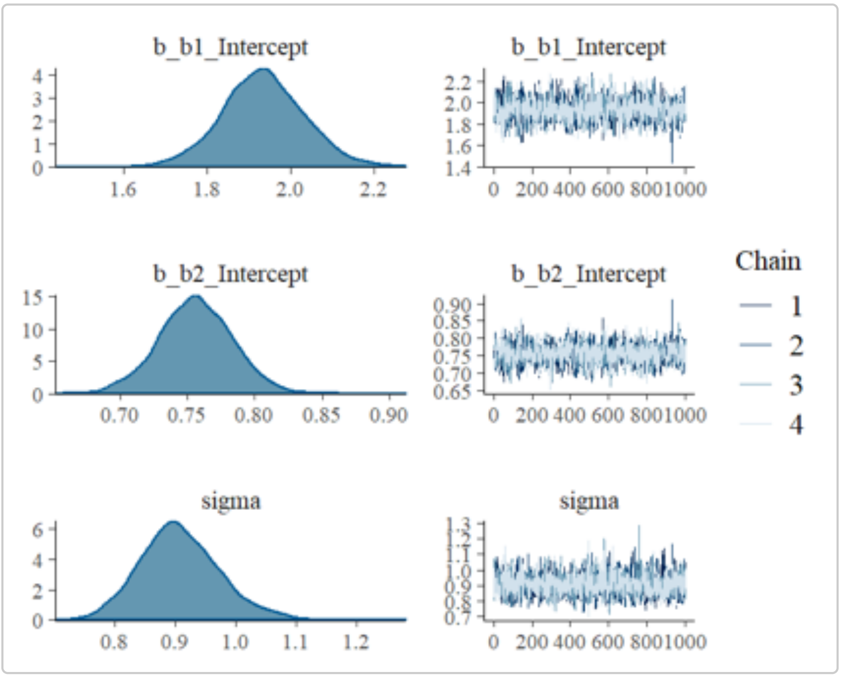
To obtain summaries of the fitted model, we apply

```
summary(fit1)
```

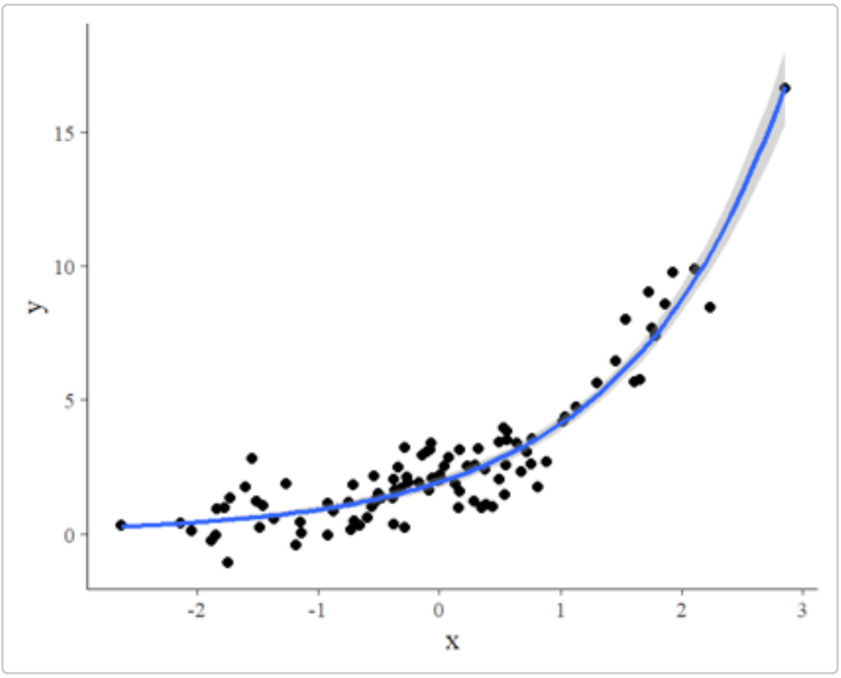
```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: y ~ b1 * exp(b2 * x)
         b1 ~ 1
         b2 ~ 1
   Data: dat1 (Number of observations: 100)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000

Population-Level Effects:
             Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
b1_Intercept     1.93      0.10     1.74     2.13       1411 1.00
```

```
b2_Intercept     0.76      0.03      0.70      0.81        1398 1.00

Family Specific Parameters:
      Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
sigma     0.91      0.07     0.79     1.05       2081 1.00

Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample
is a crude measure of effective sample size, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

```
plot(fit1)
```



```
plot(marginal_effects(fit1), points = TRUE)
```



The `summary` method reveals that we were able to recover the true parameter values pretty nicely. According to the `plot` method, our MCMC chains have converged well and to the same posterior. The `marginal_effects` method visualizes the model-implied (non-linear) regression line.

We might be also interested in comparing our non-linear model to a classical linear model.

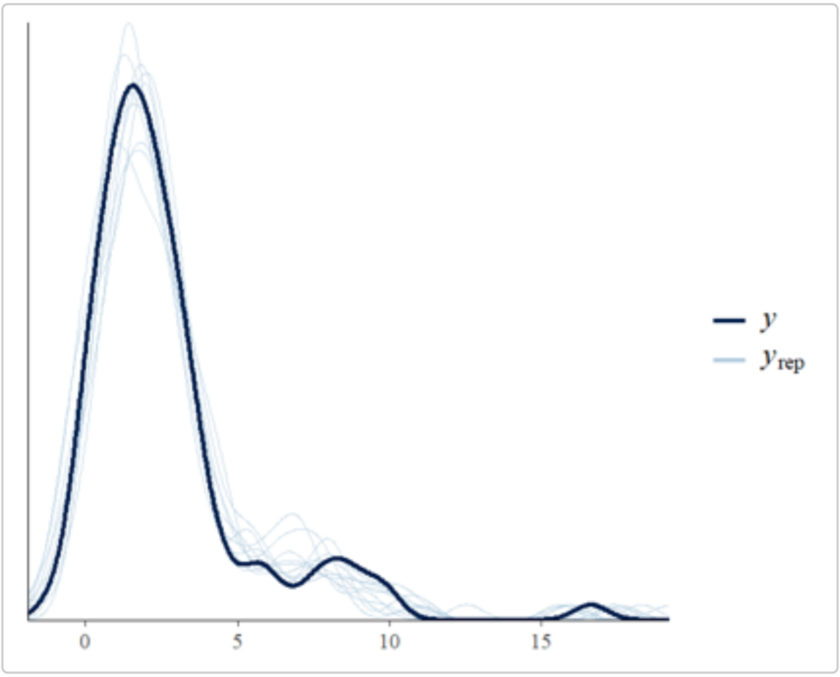
```
fit2 <- brm(y ~ x, data = dat1)
```

```
summary(fit2)
```

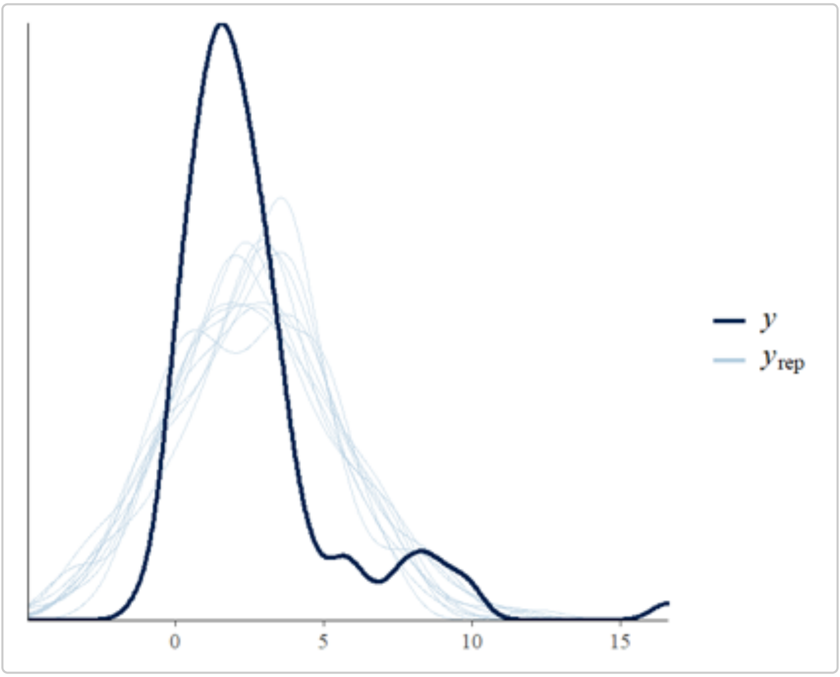
```
 Family: gaussian 
  Links: mu = identity; sigma = identity 
Formula: y ~ x 
   Data: dat1 (Number of observations: 100) 
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000

Population-Level Effects: 
          Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
Intercept     2.73      0.16     2.43     3.05       3784 1.00
x             2.01      0.15     1.72     2.30       4181 1.00

Family Specific Parameters: 
      Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
sigma     1.60      0.12     1.39     1.85       3759 1.00

Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample 
is a crude measure of effective sample size, and Rhat is the potential 
scale reduction factor on split chains (at convergence, Rhat = 1).
```

To investigate and compare model fit, we can apply graphical posterior predictive checks, which make use of the **bayesplot** package on the backend.

```
pp_check(fit1)
```



```
pp_check(fit2)
```



We can also easily compare model fit using leave-one-out cross-validation.

```
loo(fit1, fit2)
```

```
Output of model 'fit1':
```

```
Computed from 4000 by 100 log-likelihood matrix

         Estimate   SE
elpd_loo   -133.3  6.6
p_loo         3.2  0.9
looic       266.6 13.3
------
Monte Carlo SE of elpd_loo is 0.1.

Pareto k diagnostic values:
                         Count Pct.    Min. n_eff
(-Inf, 0.5]   (good)     99    99.0%   950
 (0.5, 0.7]   (ok)        1     1.0%   787
   (0.7, 1]   (bad)       0     0.0%   <NA>
   (1, Inf)   (very bad)  0     0.0%   <NA>

All Pareto k estimates are ok (k < 0.7).
See help('pareto-k-diagnostic') for details.

Output of model 'fit2':

Computed from 4000 by 100 log-likelihood matrix

         Estimate   SE
elpd_loo   -192.8 16.8
p_loo         7.7  5.3
looic       385.6 33.6
------
Monte Carlo SE of elpd_loo is NA.

Pareto k diagnostic values:
                         Count Pct.    Min. n_eff
(-Inf, 0.5]   (good)     99    99.0%   2881
 (0.5, 0.7]   (ok)        0     0.0%   <NA>
   (0.7, 1]   (bad)       0     0.0%   <NA>
   (1, Inf)   (very bad)  1     1.0%   30
See help('pareto-k-diagnostic') for details.

Model comparisons:
     elpd_diff se_diff
fit1   0.0       0.0
fit2 -59.5      17.0
```

Since smaller `LOOIC` values indicate better model fit, it is immediately evident that the non-linear model fits the data better, which is of course not too surpirsing since we simulated the data from exactly that model.

A Real-World Non-Linear model

On his blog, Markus Gesmann predicts the growth of cumulative insurance loss payments over time, originated from different origin years (see http://www.magesblog.com/post/2015/11/loss-developments-via-growth-curves-and.html). We will use a slightly simplified version of his model for demonstration purposes here. It looks as follows:

$$cum_{AY,dev} \sim N(\mu_{AY,dev}, \sigma)$$

$$\mu_{AY,dev} = ult_{AY} \left(1 - \exp\left(-\left(\frac{dev}{\theta}\right)^{\omega}\right)\right)$$

The cumulative insurance payments cum will grow over time, and we model this dependency using the variable dev. Further, ult_{AY} is the (to be estimated) ultimate loss of accident each year. It constitutes a non-linear parameter in our framework along with the parameters θ and ω, which are responsible for the growth of the cumulative loss and are assumed to be the same across years. We load the data

```
loss <- read.csv("https://paul-buerkner.github.io/data/loss.csv")
head(loss)
```

```
    AY dev      cum premium
1 1991   6  357.848   10000
2 1991  18 1124.788   10000
3 1991  30 1735.330   10000
4 1991  42 2182.708   10000
5 1991  54 2745.596   10000
6 1991  66 3319.994   10000
```

and translate the proposed model into a non-linear **brms** model.

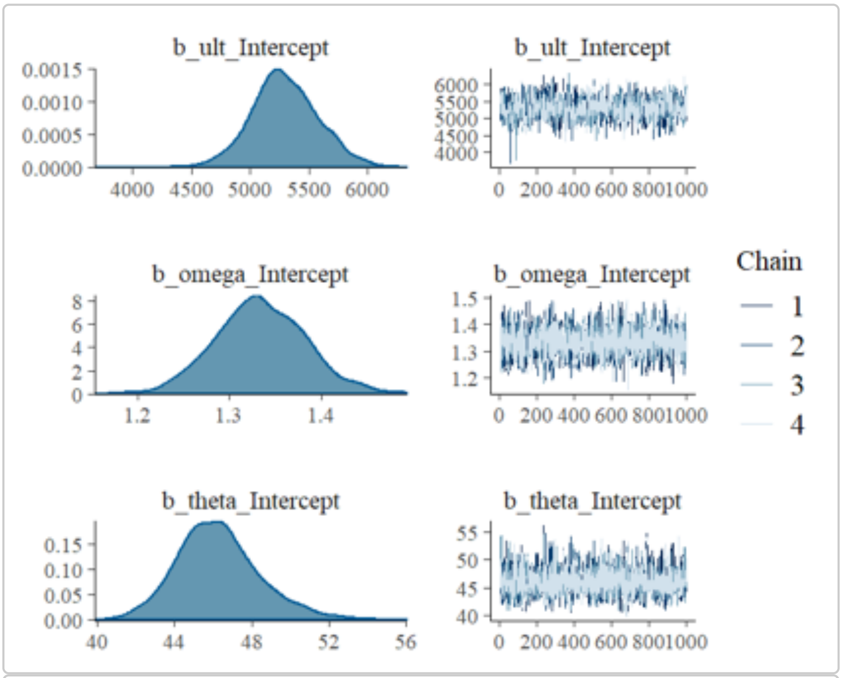
```
fit_loss <- brm(
  bf(cum ~ ult * (1 - exp(-(dev/theta)^omega)),
     ult ~ 1 + (1|AY), omega ~ 1, theta ~ 1,
     nl = TRUE),
  data = loss, family = gaussian(),
  prior = c(
    prior(normal(5000, 1000), nlpar = "ult"),
    prior(normal(1, 2), nlpar = "omega"),
    prior(normal(45, 10), nlpar = "theta")
  ),
  control = list(adapt_delta = 0.9)
)
```

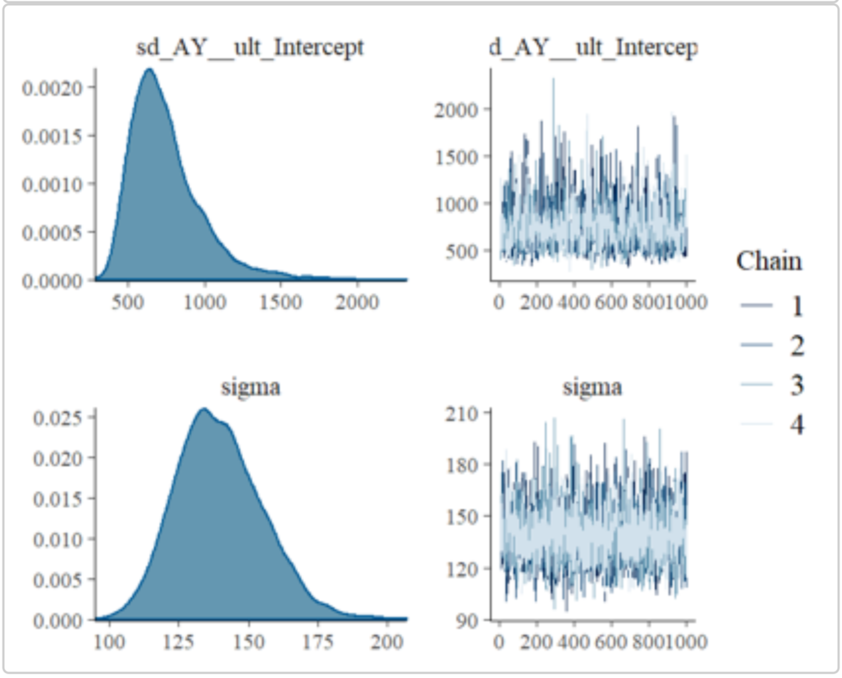
We estimate a group-level effect of accident year (variable `AY`) for the ultimate loss `ult`. This also shows nicely how a non-linear parameter is actually a placeholder for a linear predictor, which in case of `ult`, contains only an varying intercept over year. Again, priors on population-level effects are required and, for the present model, are actually mandatory to ensure identifiability. We summarize the model using well known methods.

```
summary(fit_loss)
```

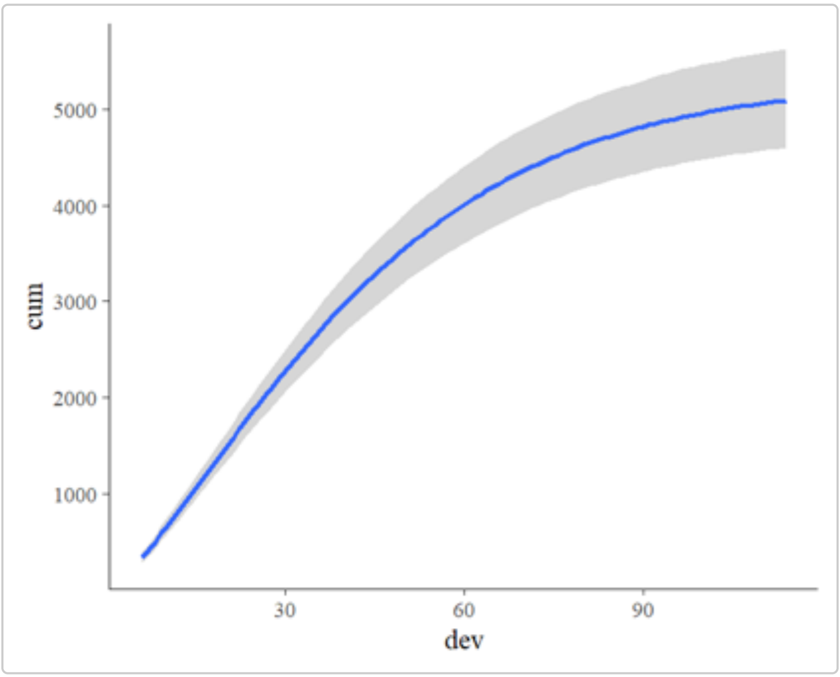
```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: cum ~ ult * (1 - exp(-(dev/theta)^omega))
         ult ~ 1 + (1 | AY)
         omega ~ 1
         theta ~ 1
   Data: loss (Number of observations: 55)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000

Group-Level Effects:
~AY (Number of levels: 10)
                  Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
sd(ult_Intercept)   747.97    230.97   437.33  1348.93       1259 1.00

Population-Level Effects:
                Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
ult_Intercept    5294.34    287.43  4739.66  5882.06        979 1.00
omega_Intercept     1.33      0.05     1.24     1.44       2388 1.00
theta_Intercept    46.29      2.18    42.34    51.16       2329 1.00

Family Specific Parameters:
      Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
sigma   139.77     15.62   112.33   172.15       2651 1.00

Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample
is a crude measure of effective sample size, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

```
plot(fit_loss, N = 3, ask = FALSE)
```



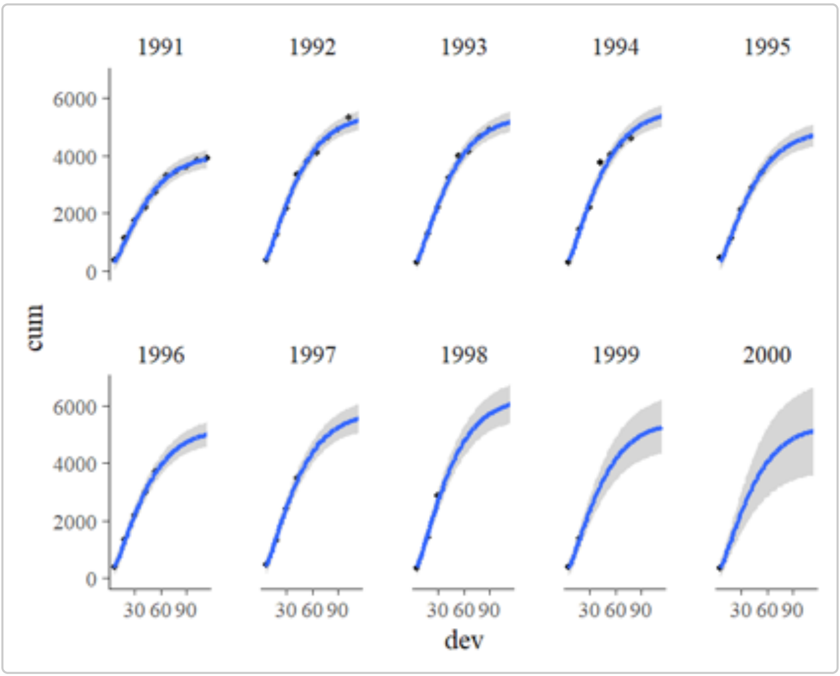


```r
marginal_effects(fit_loss)
```



Next, we show marginal effects separately for each year.

```
conditions <- data.frame(AY = unique(loss$AY))
rownames(conditions) <- unique(loss$AY)
me_loss <- marginal_effects(
  fit_loss, conditions = conditions,
  re_formula = NULL, method = "predict"
)
plot(me_loss, ncol = 5, points = TRUE)
```



It is evident that there is some variation in cumulative loss across accident years, for instance due to natural disasters happening only in certain years. Further, we see that the uncertainty in the predicted cumulative loss is larger for later years with fewer available data points.

Advanced Item-Response Models

As a third example, we want to show how to model more advanced item-response models using the non-linear model framework of **brms**. For simplicity, suppose we have a single forced choice item with three alternatives of which only one is correct. Our response variable is whether a person answers the item correctly (1) or not (0). Person are assumed to vary in their ability to answer the item correctly. However, every person has a 33% chance of getting the item right just by guessing. We thus simulate some data to reflect this situation.

```
inv_logit <- function(x) 1 / (1 + exp(-x))
ability <- rnorm(300)
p <- 0.33 + 0.67 * inv_logit(ability)
answer <- ifelse(runif(300, 0, 1) < p, 1, 0)
dat_ir <- data.frame(ability, answer)
```

The most basic item-response model is equivalent to a simple logistic regression model.

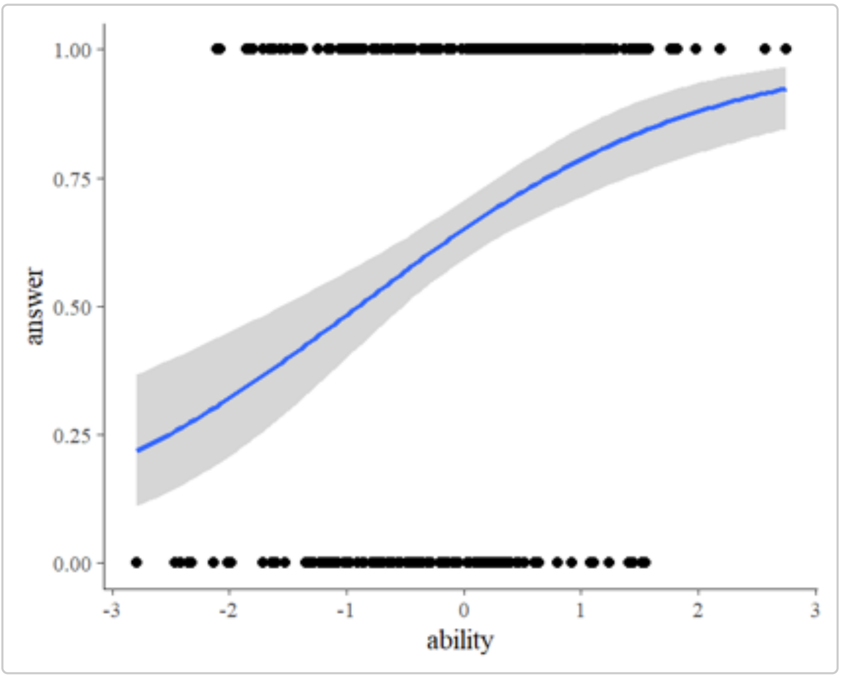
```
fit_ir1 <- brm(answer ~ ability, data = dat_ir, family = bernoulli())
```

However, this model completely ignores the guessing probability and will thus likely come to biased estimates and predictions.

```
summary(fit_ir1)
```

```
 Family: bernoulli
  Links: mu = logit
Formula: answer ~ ability
   Data: dat_ir (Number of observations: 300)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000

Population-Level Effects:
          Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
Intercept     0.62      0.13     0.37     0.87       3235 1.00
ability       0.69      0.14     0.42     0.96       3447 1.00

Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample
is a crude measure of effective sample size, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

```
plot(marginal_effects(fit_ir1), points = TRUE)
```



A more sophisticated approach incorporating the guessing probability looks as follows:

```
fit_ir2 <- brm(
  bf(answer ~ 0.33 + 0.67 * inv_logit(eta),
     eta ~ ability, nl = TRUE),
  data = dat_ir, family = bernoulli("identity"),
  prior = prior(normal(0, 5), nlpar = "eta")
)
```

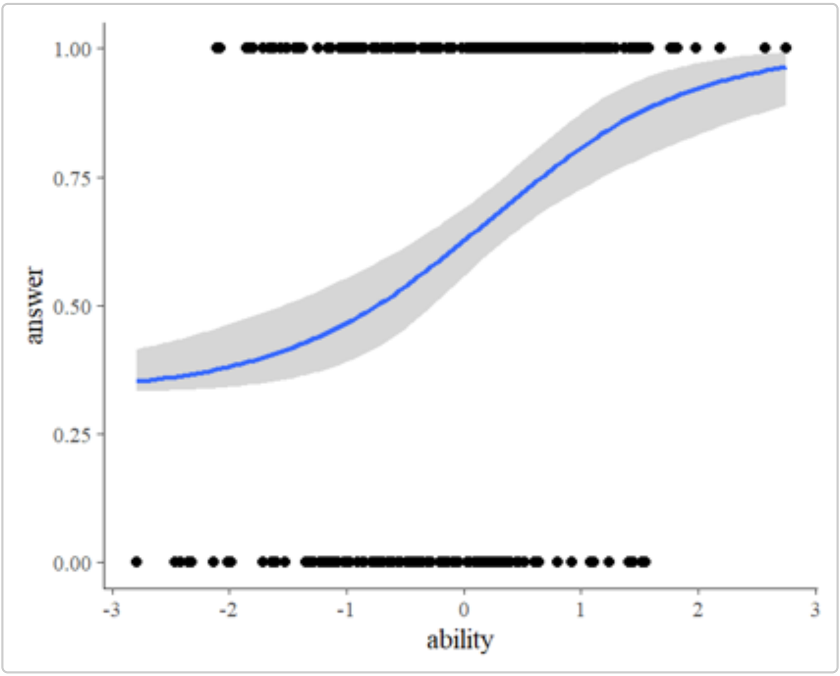
It is very important to set the link function of the `bernoulli` family to `identity` or else we will apply two link functions. This is because our non-linear predictor term already contains the desired link function (`0.33 + 0.67 * inv_logit`), but the `bernoulli` family applies the default `logit` link on top of it. This will of course lead to strange and uninterpretable results. Thus, please make sure that you set the link function to `identity`, whenever your non-linear predictor term already contains the desired link function.

```
summary(fit_ir2)
```

```
 Family: bernoulli
  Links: mu = identity
Formula: answer ~ 0.33 + 0.67 * inv_logit(eta)
         eta ~ ability
   Data: dat_ir (Number of observations: 300)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000

Population-Level Effects:
              Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
eta_Intercept    -0.25      0.21    -0.67     0.14       2010 1.00
eta_ability       1.15      0.28     0.66     1.77       2083 1.00
```

```
Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample
is a crude measure of effective sample size, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

```
plot(marginal_effects(fit_ir2), points = TRUE)
```



Comparing model fit via leave-one-out cross-validation

```
loo(fit_ir1, fit_ir2)
```

```
Output of model 'fit_ir1':

Computed from 4000 by 300 log-likelihood matrix

         Estimate   SE
elpd_loo   -185.7  6.5
p_loo         2.1  0.2
looic       371.3 13.0
------
Monte Carlo SE of elpd_loo is 0.0.

All Pareto k estimates are good (k < 0.5).
See help('pareto-k-diagnostic') for details.

Output of model 'fit_ir2':

Computed from 4000 by 300 log-likelihood matrix

         Estimate   SE
elpd_loo   -185.4  6.7
```

```
p_loo         2.2  0.2
looic       370.9 13.3
------
Monte Carlo SE of elpd_loo is 0.0.

All Pareto k estimates are good (k < 0.5).
See help('pareto-k-diagnostic') for details.

Model comparisons:
        elpd_diff se_diff
fit_ir2  0.0       0.0
fit_ir1 -0.2       1.2
```

shows that both model fit the data equally well, but remember that predictions of the first model might still be misleading as they may well be below the guessing probability for low ability values. Now, suppose that we don't know the guessing probability and want to estimate it from the data. This can easily be done changing the previous model just a bit.

```
fit_ir3 <- brm(
  bf(answer ~ guess + (1 - guess) * inv_logit(eta),
    eta ~ 0 + ability, guess ~ 1, nl = TRUE),
  data = dat_ir, family = bernoulli("identity"),
  prior = c(
    prior(normal(0, 5), nlpar = "eta"),
    prior(beta(1, 1), nlpar = "guess", lb = 0, ub = 1)
  )
)
```

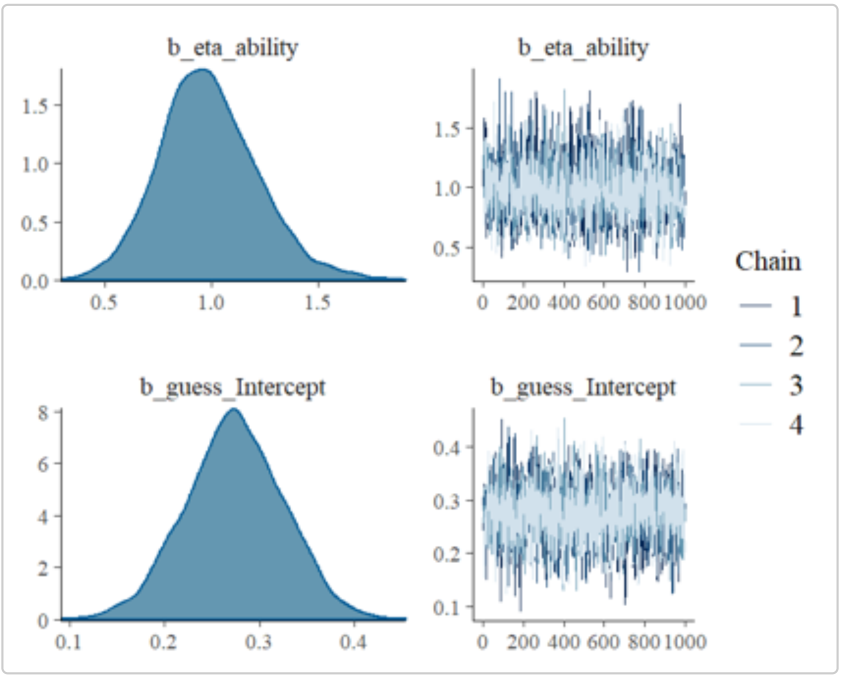
Here, we model the guessing probability as a non-linear parameter making sure that it cannot exceed the interval $[0, 1]$. We did not estimate an intercept for `eta`, as this will lead to a bias in the estimated guessing parameter (try it out; this is an excellent example of how careful one has to be in non-linear models).

```
summary(fit_ir3)
```

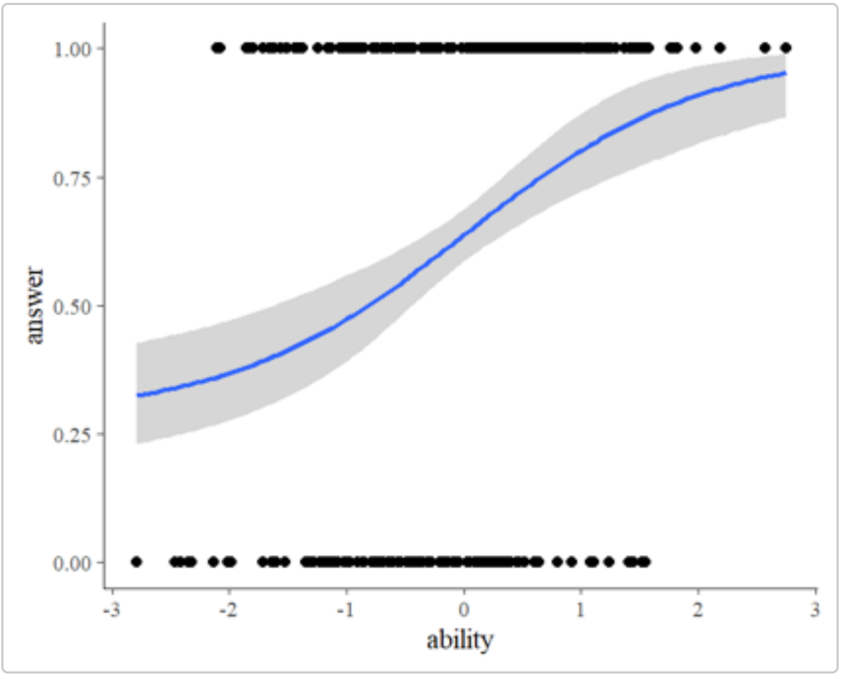
```
 Family: bernoulli
  Links: mu = identity
Formula: answer ~ guess + (1 - guess) * inv_logit(eta)
         eta ~ 0 + ability
         guess ~ 1
   Data: dat_ir (Number of observations: 300)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000

Population-Level Effects:
                Estimate Est.Error l-95% CI u-95% CI Eff.Sample Rhat
eta_ability         0.99      0.23     0.57     1.48       2294 1.00
guess_Intercept     0.27      0.05     0.17     0.37       2418 1.00
```

```
Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample
is a crude measure of effective sample size, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

```r
plot(fit_ir3)
```



```r
plot(marginal_effects(fit_ir3), points = TRUE)
```



The results show that we are able to recover the simulated model parameters with this non-linear model. Of course, real item-response data have multiple items so that accounting for item and person variability (e.g., using a multilevel model with varying intercepts) becomes necessary as we have multiple observations per item and person. Luckily, this can all be done within the non-linear framework of **brms** and I hope that this vignette serves as a good starting point.