Class 6: Partial pooling, zero-inflation, and multinomial models

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Learning outcomes:

- Be able to describe the advantages of partial pooling
- Be able to fit some basic zero inflation and hurdle models
- Be able to understand and fit some multinomial modelling examples

- For this lecture we are going to switch to Stan

A false dichotomy: fixed vs random effects

- We've been fitting a model with varying intercepts and slopes to the earnings data:

$$y_i \sim N(\alpha_{\text{eth}_i} + \beta_{\text{eth}_i} x_i, \sigma^2)$$

  where:

$$\alpha_j \sim N(\mu_\alpha, \sigma_\alpha^2) \text{ and } \beta_j \sim N(\mu_\beta, \sigma_\beta^2)$$

- In traditional parlance this is a random effects model
- When we fit our model we are learning about the values of the slopes and intercepts, and also the values of their means and standard deviations

The extremes of varying vs fixed parameters

- Now consider what happens when σ_α and σ_β get smaller and smaller. What will happen to the values of the slopes and the intercepts?
- Alternatively, consider what happens as σ_α and σ_β get larger and larger?
- Are these still random effects models?

The advantages of borrowing strength

- The process of σ_α and σ_β getting smaller or larger will control the degree to which the slopes and intercepts are similar to each other
- If they are similar to each other we say they are *borrowing strength* as data in the other groups is influencing the intercept/slope. This is a powerful idea
- Mathematically you can write out the estimated mean of the parameters as a weighted average of the group mean and the overall mean where the weights are dependent on the group and overall variance and sample sizes.
- Because of the weighted nature of the estimate this is often called *partial pooling*

Zero-inflation and hurdle models

- Let's introduce some new data. This is data from an experiment on whiteflies:

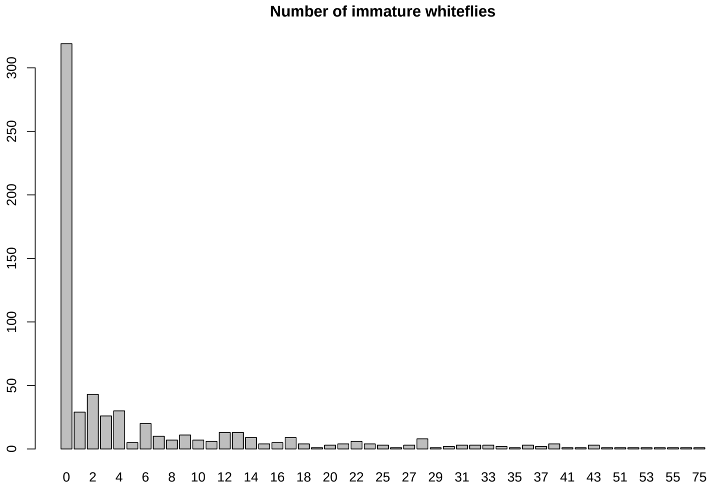
```r
wf = read.csv('../data/whitefly.csv')
head(wf)
```

```
##   imm week block trt  n live plantid
## 1  15    1     3   5 12   11       1
## 2  16    2     3   5  8    6       1
## 3  28    3     3   5 10   10       1
## 4  17    4     3   5 10    8       1
## 5   9    5     3   5 10   10       1
## 6  28    6     3   5 10   10       1
```

The response variable here is the count `imm` of immature whiteflies, and the explanatory variables are `block` (plant number), `week`, and treatment `treat`.

Look at those zeros!

```
barplot(table(wf$imm),
        main = 'Number of immature whiteflies')
```



A first model

- These are count data so a Poisson distribution is a good start
- Let's consider a basic Poisson distribution model for Y_i, $i = 1, \ldots, N$ observations:

$$Y_i \sim Po(\lambda_i)$$

$$\log(\lambda_i) = \beta_{\mathsf{trt}_i}$$

- We'll only consider the treatment effect but we could run much more complicated models with e.g. other covariates and interactions

Fitting the model in Stan

```
stan_code = '
data {
  int<lower=0> N;
  int<lower=0> N_trt;
  int<lower=0> y[N];
  int trt[N];
}
parameters {
  real beta_trt[N_trt];
  real trt_mean;
  real<lower=0> trt_sd;
}
model {
  for (i in 1:N)
    y[i] ~ poisson_log(beta_trt[trt[i]]);

  # Priors on coefficients
  for(j in 1:N_trt)
    beta_trt[j] ~ normal(trt_mean, trt_sd);

  trt_mean ~ normal(0, 10);
  trt_sd ~ cauchy(0, 5);
}
'
```

Running the model

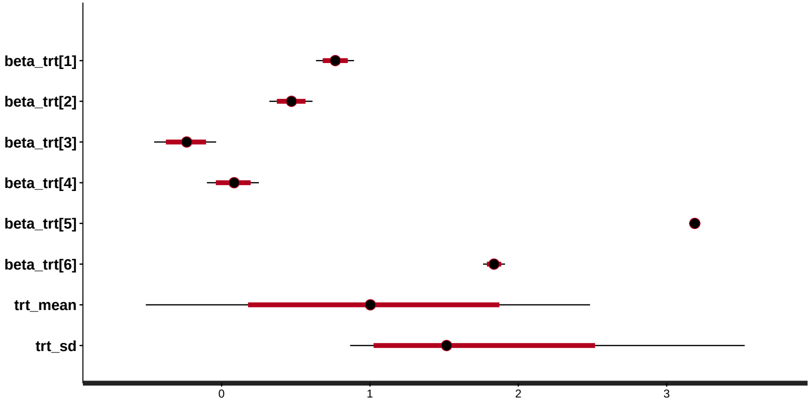
```
stan_run = stan(data = list(N = nrow(wf),
                            N_trt = length(unique(wf$trt)),
                            y = wf$imm,
                            trt = wf$trt),
                model_code = stan_code)
```

Results

```
plot(stan_run)
```

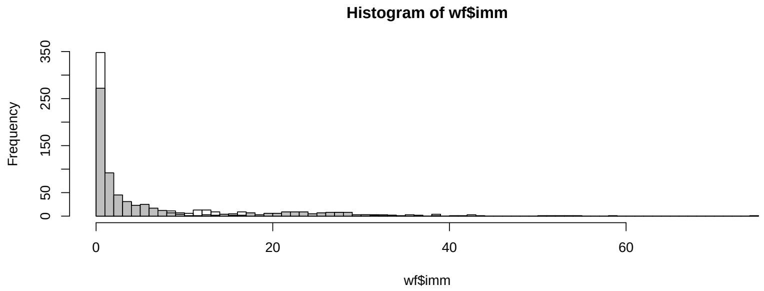
```
## ci_level: 0.8 (80% intervals)

## outer_level: 0.95 (95% intervals)
```



Did the model actually fit well?

```
pars = extract(stan_run, pars = 'beta_trt')$beta_trt
beta_means = apply(pars,2,'mean')
y_sim_mean = exp(beta_means[wf$trt])
y_sim = rpois(nrow(wf), y_sim_mean)
hist(wf$imm, breaks = seq(0,max(wf$imm)))
hist(y_sim, breaks = seq(0,max(wf$imm)),
     add = TRUE, col = 'gray')
```



What about the zeros?

- One way of broadening the distribution is through over-dispersion which we have already met:

$$\log(\lambda_i) \sim N(\beta_{\text{trt}_i}, \sigma^2)$$

- However this doesn't really solve the problem of excess zeros
- Instead there are a specific class of models called *zero-inflation* models which use a specific probability distribution. The zero-inflated Poisson (ZIP) with ZI parameter q_0 is written as:

$$p(y|\lambda) = \begin{cases} q_0 + (1 - q_0) \times \mathit{Poisson}(0, \lambda) & \text{if } y = 0 \\ (1 - q_0) \times \mathit{Poisson}(y, \lambda) & \text{if } y = 0 \end{cases}$$

Fitting models with custom probability distributions

- The Zero-inflated Poisson distribution is not included in Stan or JAGS by default. We have to create it
- It's pretty easy to create new probability distributions in Stan
- It's quite hard to do so in JAGS, requiring some weird tricks
- In Stan all of you have to do is give it a way of computing the likelihood score, which it keeps track of via a variable called `target`

Fitting the ZIP in Stan

```
stan_code = '
data {
  int<lower=0> N;
  int<lower=0> N_trt;
  int<lower=0> y[N];
  int trt[N];
}
parameters {
  real<lower=0, upper=1> q_0;
  real beta_trt[N_trt];
  real trt_mean;
  real<lower=0> trt_sd;
}
model {
  for(j in 1:N_trt)
    beta_trt[j] ~ normal(trt_mean, trt_sd);
  trt_mean ~ normal(0, 10);
  trt_sd ~ cauchy(0, 5);

  for (i in 1:N) {
    if (y[i] == 0)
      target += log_sum_exp(bernoulli_lpmf(1 | q_0),
                                bernoulli_lpmf(0 | q_0)
                                  + poisson_log_lpmf(y[i] | beta_trt[trt[i]]));
    else
      target += bernoulli_lpmf(0 | q_0) + poisson_log_lpmf(y[i] | beta_trt[trt[i]]);
  }
}
'
```

Running the model

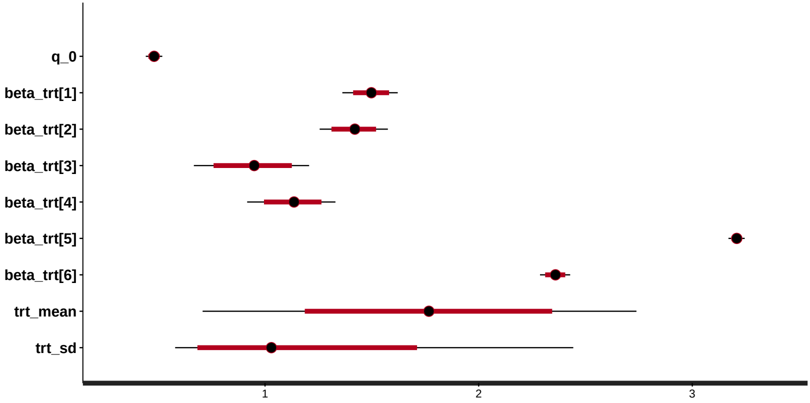
```
stan_run = stan(data = list(N = nrow(wf),
                            N_trt = length(unique(wf$trt)),
                            y = wf$imm,
                            trt = wf$trt),
                model_code = stan_code)
```

Results

```
plot(stan_run)
```

```
## ci_level: 0.8 (80% intervals)

## outer_level: 0.95 (95% intervals)
```

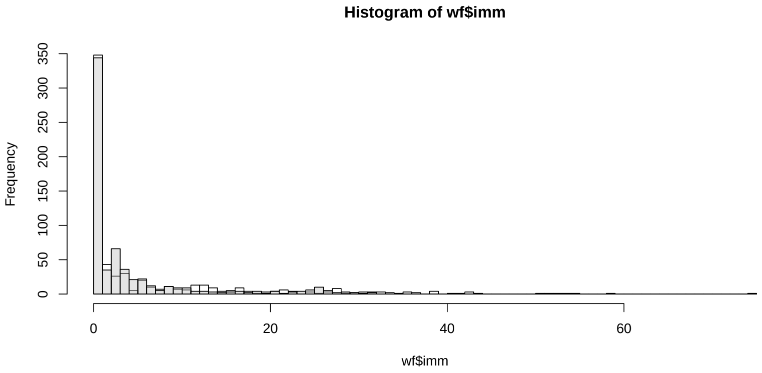


Did it work any better? - code

```
beta_means = apply(extract(stan_run, pars = 'beta_trt')$bet
q_0_mean = mean(extract(stan_run, pars = 'q_0')$q_0)
y_sim_mean = exp(beta_means[wf$trt])
rZIP = function(mean, q_0) {
  pois = rpois(length(mean), mean)
  pois[runif(length(mean))<q_0] = 0
  return(pois)
}
y_sim = rZIP(y_sim_mean, q_0_mean)
```

Did it work any better? - picture

```
hist(wf$imm, breaks = seq(0,max(wf$imm)))
hist(y_sim, breaks = seq(0,max(wf$imm)),
     add = TRUE, col = rgb(0.75,0.75,0.75,0.4))
```



Some more notes on Zero-inflated Poisson

- This model seems to over-predict the number of zeros! It would be interesting to perhaps try having a different probability of zeros (q_0) for different treatments
- It might be that the other covariates explain some of the zero behaviour
- We could further add in both zero-inflation and over-dispersion

An alternative: hurdle models

- ZI models work by having a parameter (here q_0) which is the probability of getting a zero, and so the probability of getting a Poisson value (which could also be a zero) is 1 minus this value
- An alternative (which is slightly more complicated) is a hurdle model where q_0 represents the probability of the *only way* of getting a zero. With probability (1-q_0) we end up with a special Poisson random variable which has to take values 1 or more
- In some ways this is richer than a ZI model since zeros can be deflated or inflated

A hurdle-Poisson model in Stan

```
stan_code = '
data {
  int<lower=0> N;
  int<lower=0> N_trt;
  int<lower=0> y[N];
  int trt[N];
}
parameters {
  real<lower=0, upper=1> q_0;
  real beta_trt[N_trt];
  real trt_mean;
  real<lower=0> trt_sd;
}
model {
  for(j in 1:N_trt)
    beta_trt[j] ~ normal(trt_mean, trt_sd);
  trt_mean ~ normal(0, 10);
  trt_sd ~ cauchy(0, 5);

  for (i in 1:N) {
    if (y[i] == 0)
          target += log(q_0);
        else
          target += log1m(q_0) + poisson_log_lpmf(y[i] | beta_trt[trt[i]])
                    - poisson_lccdf(0 | exp(beta_trt[trt[i]]));
  }
}
'
```

Running the model

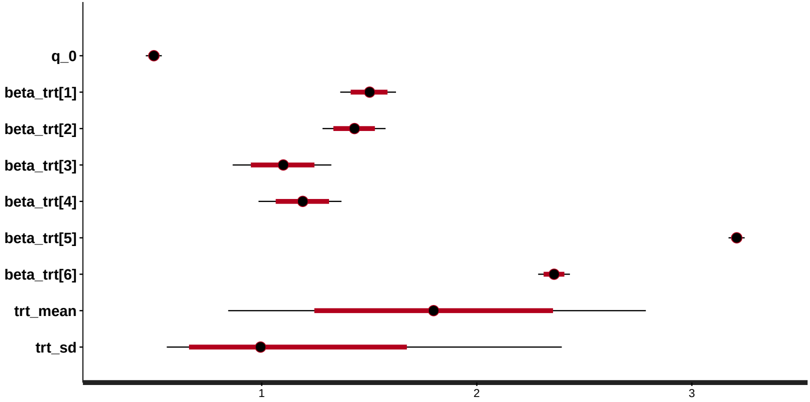
```r
stan_run = stan(data = list(N = nrow(wf),
                            N_trt = length(unique(wf$trt))
                            y = wf$imm,
                            trt = wf$trt),
                model_code = stan_code)
```

Results

```r
plot(stan_run)
```

```
## ci_level: 0.8 (80% intervals)
```

```
## outer_level: 0.95 (95% intervals)
```

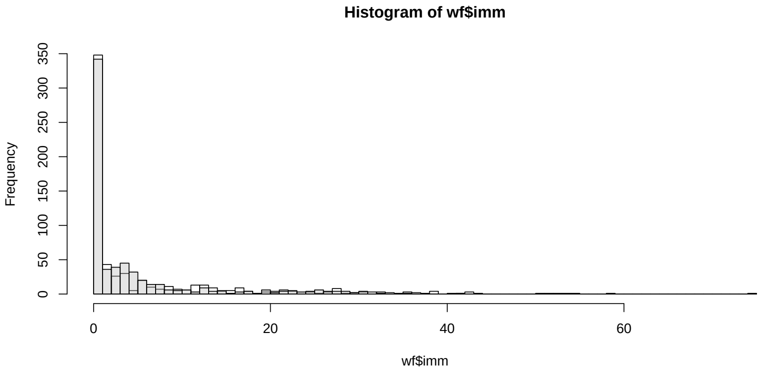


Did it work any better? - code

```
beta_means = apply(extract(stan_run, pars = 'beta_trt')$bet
q_0_mean = mean(extract(stan_run, pars = 'q_0')$q_0)
y_sim_mean = exp(beta_means[wf$trt])
rZIP = function(mean, q_0) {
  pois = rpois(length(mean), mean)
  pois[runif(length(mean))<q_0] = 0
  return(pois)
}
y_sim = rZIP(y_sim_mean, q_0_mean)
```

Did it work any better? - picture

```r
hist(wf$imm, breaks = seq(0,max(wf$imm)))
hist(y_sim, breaks = seq(0,max(wf$imm)),
     add = TRUE, col = rgb(0.75,0.75,0.75,0.4))
```



The multinomial distribution

- Multinomial data can be thought of as multivariate discrete data
- It's usually used in two different scenarios:
  1. For classification, when you have an observation falling into a single one of K possible categories
  2. For multinomial regression, where you have a set of counts which sum to a known value N
- We will just consider the multinomial regression case, whereby we have observations $y_i = [y_{i1}, \ldots, y_{iK}]$ where the sum $\sum_{k=1}^{K} y_{ik} = N_i$ is fixed
- The classification version is a simplification of the regression version

Some new data! - pollen

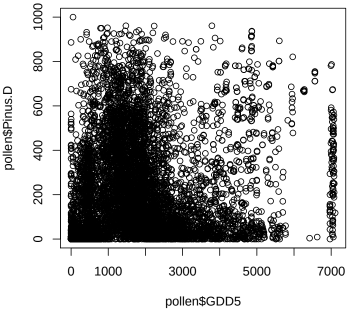
```r
pollen = read.csv('../data/pollen.csv')
head(pollen)
```

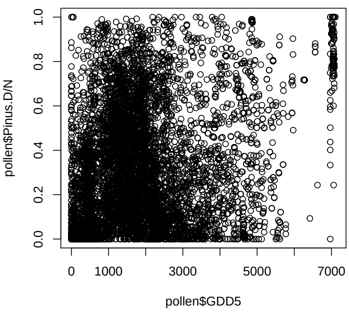
```
##   GDD5 MTCO Abies Alnus Betula Picea Pinus.D Quercus.D C
## 1 1874 -7.9     0    50    158     7     721        22
## 2 1623 -5.5     0    38     28   302     537        19
## 3 1475 -4.7     0   276    183   110     136         0
## 4 1360 -8.8     0   111    354   141     364         0
## 5 1295 -6.9     0    91     50   151     708         0
## 6 1539 -7.8     0    51    194    82     673         0
```

These data are pollen counts of 7 varieties of pollen from modern samples with two covariates

Some plots

- The two covariates represent the length of the growing season (GDD5) and harshness of the winter (MTCO)
- The task is to find which climate regimes each pollen variety favours





A multinomial model

- The multinomial distribution is often written as:

$$[y_{i1}, \ldots, y_{iK}] \sim Mult(N_i, \{p_{i1}, \ldots, p_{iK}\})$$

  or, for short:

$$y_i \sim Mult(N_i, p_i)$$

- The key parameters here are the probability vectors p_i. It's these we want to use a link function on to include the covariates
- We need to be careful as each must sum to one: $\sum_{k=1}^{K} p_{ik} = 1$. Any link function must satisfy this constraint

Prior distributions on probability vectors

- When $K = 2$ we're back the binomial-logit we met in the first day, and we can use the logit link function
- When $K > 2$ a common function to use is the *soft-max* function:
$$p_{ik} = \frac{\exp(\theta_{ik})}{\sum_{j=1}^{K} \exp(\theta_{ij})}$$
- This is a generalisation of the logit function
- The next layer of our model sets, e.g.:

$$\theta_{ik} = \alpha_k + \beta_k \text{GDD5} + \gamma_k \text{MTCO}$$

Stan code part 1

```
stan_code = '
data {
  int<lower=1> n;
  int<lower=1> K;
  int<lower=0> y[n,K];
  real x1[n];
  real x2[n];
}
parameters {
  vector[K] alpha;
  vector[K] beta;
  vector[K] gamma;
  real alpha_mean;
  real beta_mean;
  real gamma_mean;
  real<lower=0> sigma_alpha;
  real<lower=0> sigma_beta;
  real<lower=0> sigma_gamma;
}
transformed parameters {
  vector[K] theta[n];
  simplex[K] p[n];

  for(i in 1:n){
    theta[i] =  alpha + beta*x1[i] + gamma*x2[i];
  }
  for(i in 1:n){
    p[i] = softmax(theta[i]);
  }
}
...
'
```

Stan code part 2

```
stan_code = '
...
model {
  for(k in 1:K) {
    alpha[k] ~ normal(alpha_mean,sigma_alpha);
    beta[k] ~ normal(beta_mean,sigma_beta);
    gamma[k] ~ normal(gamma_mean,sigma_gamma);
  }
  alpha_mean ~ normal(0, 10);
  beta_mean ~ normal(0, 10);
  gamma_mean ~ normal(0, 10);
  sigma_alpha ~ cauchy(0, 5);
  sigma_beta ~ cauchy(0, 5);
  sigma_gamma ~ cauchy(0, 5);

  for(i in 1:n)
    y[i] ~ multinomial(p[i]);
}
'
```

```
# pollen2 = pollen[sample(1:nrow(pollen), 200),]
# stan_run = stan(data = list(K = 3,
#                              n = nrow(pollen2),
#                              y = pollen2[,3:5],
#                              x1 = scale(pollen2$GDD5)[,1],
#                              x2  = scale(pollen2$MTCO)[,1]),
#                 model_code = stan_code)
```

Notes about this model

- This model is not going to fit very well, since it is unlikely that a linear relationship between the covariates and the pollen counts will match the data
- It might be better to use e.g. a spline model (not covered in this course, but we can talk about it)
- Similarly we might need some complex interactions between the covariates as they are strongly linked
- We have constrained the parameters here so that the slopes and intercepts borrow strength across species. Does this make sense? What else could we do?

Some final notes about multinomial models

- These models can be a pain to deal with as there are tricky constraints on the θ parameters to make them all sum to 1.
- The `softmax` function is one choice but there are lots of others (logistic ratios, the Dirichlet distribution, ...)
- Whilst the classification version of this model just has binary y_i (with just a single 1 in it) most packages (including JAGS and Stan) have a special distribution (e.g. `dcat` in JAGS) for this situation

Summary

- We have seen how partial pooling is a balance between a model of complete independence and complete dependence between groups
- We have fitted some zero inflated and hurdle Poisson models
- We have seen some (poorly fitting) multinomial regression models