An introduction to Generalized Linear Models (GLMs)

FW 891

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Purpose

- Introduce design matrices for linear models
- Introduce Generalized Linear Models
  - In particular, the Poisson and binomial GLMs
- Simulate fake data from these models
- Write Stan code to estimate the parameters of these models
- A fun question

Breaking statistical models down

response = deterministic component + random component

- This section / lecture is based heavily on Kery and Schaub 2012; Kery and Royle 2016

The random (noise) component

- Hallmark of statistical models: they must account for randomness
- Check out ?d*dist* in R, and replace *dist* by any of the following: pois, binom, norm, multinom, exp, and unif
- Changing first letter d to p, q, or r allows one to get the density, the distribution function, the percentiles, and random numbers from these distributions, respectively.
  - Note R calls mass functions density functions (e.g., `dbinom()`)

Kery and Schaub 2012; Kery and Royle 2016

The deterministic (signal) component

- The signal component of the model contains the predictable parts of a response or the mean structure of a model
- Often the mean structure is described by a linear model, although nonlinear models can also be used (Seber and Wild 2003)
- Linear model is just one specific way to describe how we imagine our explantory variables influencing our repsonse
- This model is linear in the parameters and does not need to represent a straight line when plotted
- t-test, simple and multiple linear regressions, ANOVA, ANCOVA, and many mixed models are all linear models

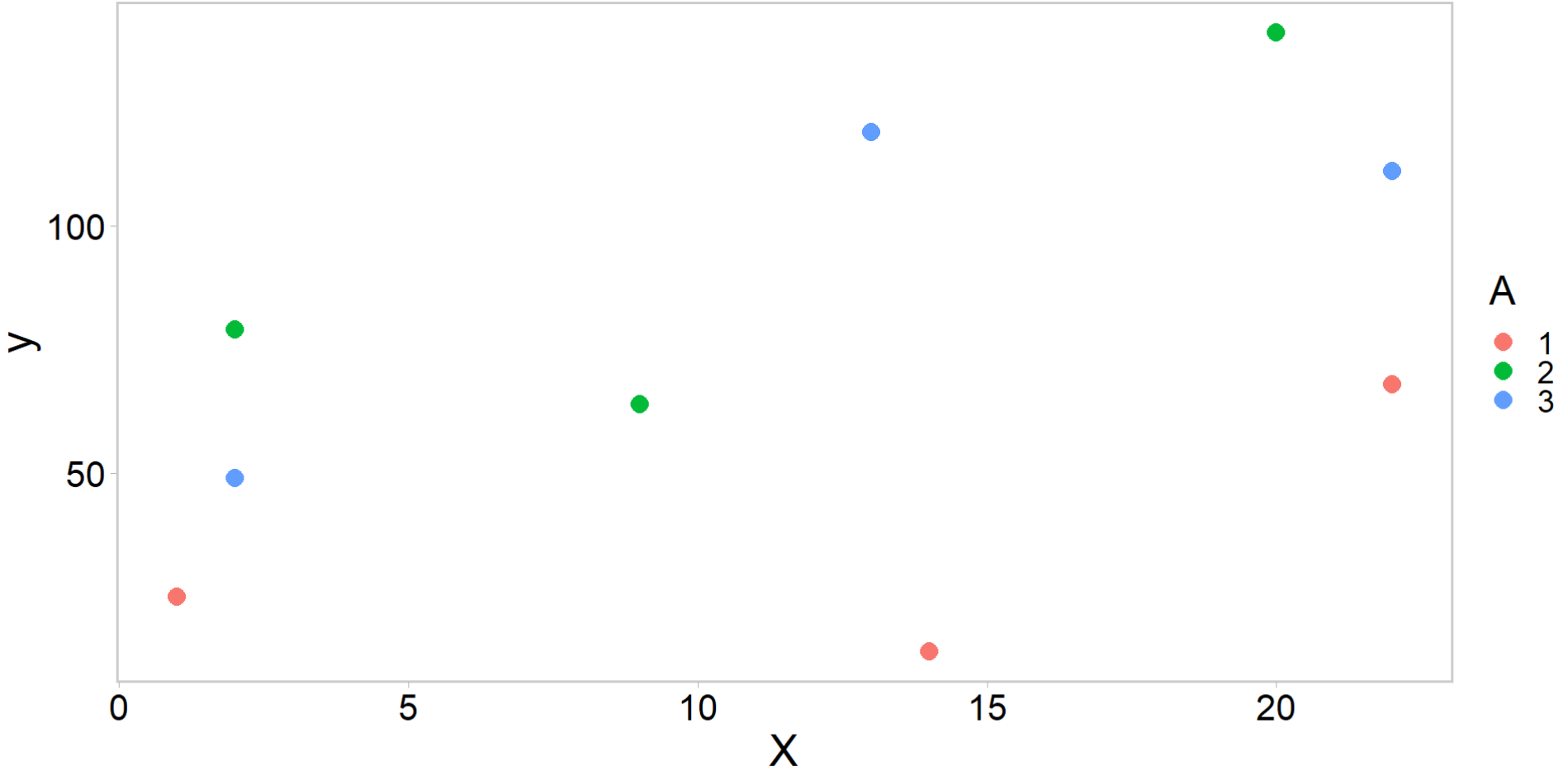
Kery and Schaub 2012; Kery and Royle 2016

A brief illustration of an analysis of covariance ANCOVA

```r
library(tidyverse)
library(ggqfc)
y <- c(25, 14, 68, 79, 64, 139, 49, 119, 111) # obs
A <- factor(c(1, 1, 1, 2, 2, 2, 3, 3, 3)) # group
X <- c(1, 14, 22, 2, 9, 20, 2, 13, 22) # covariate
my_df <- data.frame(y, A, X)

my_df %>%
  ggplot(aes(X, y, color = A)) +
  geom_point(pch = 16, size = 3.5) + theme_qfc()
```

A brief illustration of an analysis of covariance ANCOVA



Running the (Frequentist) ANCOVA in R

```
1  lm(y ~ A - 1 + X)
```

```
Call:
lm(formula = y ~ A - 1 + X)

Coefficients:
    A1       A2       A3        X
 1.315   65.218   58.648    2.785
```

- This so-called “formula language” is clever because it is quick and error-free *if you know how to specify your model*
- What does y ~ A−1 + X actually mean?

Kery and Schaub 2012; Kery and Royle 2016

ANCOVA maths

- When we fitted that model, we were doing the following:

$$y_i = \beta_{g(i)} + \beta_1 \cdot X_i + \varepsilon_i \quad \text{where} \quad \varepsilon_i \sim \mathrm{N}\left(0, \sigma^2\right)$$

- y_i is a response of unit (data point, individual, row) i, X_i is the value of the continuous explanatory variable x for unit i
- Factor A codes for the group membership of each unit with indeces g for groups 1,2, or 3
- Two parameters in the mean relationship, $\beta_{g(i)}$ and β_1
  - First of these is a vector, second a scalar
  - Index g indicates group 1, 2, or 3

ANCOVA maths: one way

$$y_i = \beta_{g(i)} + \beta_1 \cdot X_i + \varepsilon_i \quad \text{where} \quad \varepsilon_i \sim \mathrm{N}\left(0, \sigma^2\right)$$

- The random (noise) part of the model consists of the part of the response which we cannot explain using our linear combination of explanatory variables
  - Represented by residuals ε_i
  - Assume they come from a normal distribution with common variance σ^2
- How many parameters in total does this model have?

ANCOVA maths another way

Old way:

$$y_i = \beta_{g(i)} + \beta_1 \cdot X_i + \varepsilon_i \quad \text{where} \quad \varepsilon_i \sim \mathrm{N}\left(0, \sigma^2\right)$$

Shifting the structure of the model via algebra:

$$y_i \sim \mathrm{N}\left(\beta_{g(i)} + \beta_1 \cdot X_i, \sigma^2\right).$$

ANCOVA maths even more ways

A further possibility:

$$y_i \sim \mathrm{N}\left(\mu_i, \sigma^2\right), \quad where \quad \mu_i = \beta_{g(i)} + \beta_1 \cdot X_i$$

- Being able to write a linear model in algebra helps code the model in Stan (or any other modeling platform)
- Also helps you understand commonalities between many common statistical tests and what `lm()` in R is doing

ANCOVA: but wait, there's more 🥴 🤔

The same model via matrix and vector notation:

$$\begin{pmatrix} 25 \\ 14 \\ 68 \\ 79 \\ 64 \\ 139 \\ 49 \\ 119 \\ 111 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 14 \\ 1 & 0 & 0 & 22 \\ 0 & 1 & 0 & 2 \\ 0 & 1 & 0 & 9 \\ 0 & 1 & 0 & 20 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 1 & 13 \\ 0 & 0 & 1 & 22 \end{pmatrix} \times \begin{pmatrix} \beta_{g=1} \\ \beta_{g=2} \\ \beta_{g=3} \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \\ \varepsilon_7 \\ \varepsilon_8 \\ \varepsilon_9 \end{pmatrix}, \text{with } \varepsilon_i \sim \mathrm{N}\left(0, \sigma^2\right)$$

- Left to right: response vector, design matrix, parameter vector, residual vector

ANCOVA: but wait, there's more 🥴 🤔

The same model via matrix and vector notation:

$$\begin{pmatrix} 25 \\ 14 \\ 68 \\ 79 \\ 64 \\ 139 \\ 49 \\ 119 \\ 111 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 14 \\ 1 & 0 & 0 & 22 \\ 0 & 1 & 0 & 2 \\ 0 & 1 & 0 & 9 \\ 0 & 1 & 0 & 20 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 1 & 13 \\ 0 & 0 & 1 & 22 \end{pmatrix} \times \begin{pmatrix} \beta_{g=1} \\ \beta_{g=2} \\ \beta_{g=3} \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \\ \varepsilon_7 \\ \varepsilon_8 \\ \varepsilon_9 \end{pmatrix}, \text{with } \varepsilon_i \sim \mathrm{N}\left(0, \sigma^2\right)$$

- The value of the linear predictor for the first data point is given by $1 \cdot \beta_{g=1} + 0 \cdot beta_{g=2} + 0 \cdot beta_{g=3} + 1 \cdot \beta_1$

A trick for learning about the design matrix in R: `model.matrix()`

```r
# Means parameterization
X_ij <- model.matrix(~ A - 1 + X)
X_ij # rows = i, j = columns
```

```
  A1 A2 A3  X
1  1  0  0  1
2  1  0  0 14
3  1  0  0 22
4  0  1  0  2
5  0  1  0  9
6  0  1  0 20
7  0  0  1  2
8  0  0  1 13
9  0  0  1 22
attr(,"assign")
[1] 1 1 1 2
attr(,"contrasts")
attr(,"contrasts")$A
[1] "contr.treatment"
```

- see also effects or treatment contrast parameterization `model.matrix(~ A + X)`

for more information on linear model see: Kery 2010

The ANCOVA in Stan

- The code looks very similar to the algebraic specification of this linear model
  - Note I am picking vague-ish priors but the specific priors aren't the point of this lesson

The ANCOVA.stan file

```
data {
  int<lower=0> n_obs;         // number of observations = i
  int<lower=0> n_col;         // columns of design matrix = j
  vector[n_obs] y_obs;        // observed data
  matrix[n_obs, n_col] X_ij; // design matrix: model.matrix(~A-1+X)
}
parameters {
 vector[n_col] b_j; // one parameter for each column of Xij
 real<lower=0> sig; // sigma must be postive
}
model {
  vector[n_obs] y_pred;         // container for mean response
  b_j ~ normal(0,100);          // priors for b_j
  sig ~ normal(0,100);          // prior for sig
  y_pred = X_ij * b_j;          // linear algebra sneakery
  y_obs ~ normal(y_pred, sig); // likelihood
}
```

And the corresponding R code:

```r
library(cmdstanr)
mod <- cmdstan_model("week3/soln_files/ANCOVA.stan") # compile

# names in tagged list correspond to the data block in the Stan program
X_ij <- model.matrix(~ A - 1 + X)
stan_data <- list(n_obs = nrow(X_ij), n_col = ncol(X_ij),
                  y_obs = my_df$y, X_ij = as.matrix(X_ij)
                  )

# write a function to get starting values
inits <- function() {
  list(
    b_j = jitter(rep(0, ncol(X_ij)), amount = 0.5),
    sig = jitter(10, 1)
  )
}

fit <- mod$sample(
  data = stan_data,
  init = inits,
  seed = 1, # ensure simulations are reproducible
  chains = 4, # multiple chains
  iter_warmup = 1000, # how long to warm up the chains
  iter_sampling = 1000, # how many samples after warmp
  parallel_chains = 4 # run them in parallel?
)
```

- Note this is all in the solution file for this week

Break

- Now we will move into Generalized Linear Models (GLM), where all of the information we just learned still applies
- Primary difference for GLMs is that they will allow us to model non-normal response variables in a manner similar to what we just did with an ANCOVA
  - Do this via a `link` function

Generalized Linear Models (GLMs)

- The GLM is a flexible generalization of linear regression, developed by Nelder and Wedderburn in 1972 while working together at the Rothamsted Experimental Station in the U.K.
- Extend the concept of linear effect of covariates to response variables for statistical distributions where something other than a normal is assumed
  - e.g., Poisson, binomial/Bernoulli, gamma, exponential, etc.
- Linear effect of covariates is expressed not for the expected response directly, but rather for a transformation of the expected response (McCullagh and Nelder 1989)
- Unifies various statistical methods, and thus fundamental to much contemporary statistical modeling

Hilbe et al. 2017; Gelman and Hill 2007; Kery and Royle 2016

Generalized Linear Models (GLMs)

- The linear effect of covariates is expressed not for the expected response directly, but for a transformation of the expected response (Kery and Royle 2016)
  - This transformation is called a *link* function

We generally describe a GLM for a response y_i in terms of three things:

1. A random component (i.e., the likelihood)
2. A link function (i.e., a mathematical transformation)
3. Systematic component (i.e., the linear predictor)

Hilbe et al. 2017; Gelman and Hill 2007; Kery and Royle 2016

The three parts of a GLM

1. Random component of the response: a statistical distribution f with parameter(s) θ:

$$y_i \sim f(\theta)$$

2. A link function g, which is applied to the expected response $E(y) = \mu_i$, with η_i known as the linear predictor:

$$g(E(y)) = g(\mu_i) = \eta_i$$

3. Systematic part of the response (mean structure of the model containing a linear model):

$$\eta_i = \beta_0 + \beta_1 \cdot x_i$$

see Chapter 3, Kery and Royle 2016

We can combine elements 2 and 3 and define a GLM succinctly as:

$$y_i \sim f(\theta)$$
$$g(\mu_i) = \beta_0 + \beta_1 \cdot x_i$$

- A response y follows a distribution f with parameter(s) θ, and a transformation g of the expected response, which is modeled as a linear function of covariates
- This is how we will code them in Stan, which makes the Bayesian framework powerful for learning GLMs

see Chapter 3, Kery and Royle 2016

Why you should care part I

- GLM concept gives you considerable creative freedom in combining the three components
  - However, there are typically pairs of response distributions and link functions that go well together
    - These are called *canonical* link functions
  - Identity link for normal responses: $\eta_i = \mu_i$
  - Log link for Poisson responses: $\eta_i = log(\mu_i)$
  - Logit link for binomial or Bernoulli responses: $\eta_i = log(\mu_i / (1 - \mu_i))$
- These three GLMs make up vast number of statistical methods used in ecology

see Chapter 3, Kery and Royle 2016

Why you should care part II

- Bernoulli/binomial: survival, maturity, presence/absence, data either 0 or 1
- Poisson: abundance, recruitment, unbounded counts [0, Inf]
- Many exciting ecological models can be viewed as coupled GLMs
- GLMs are defined for all members of statistical distributions belonging to the so-called “exponential family” (McCullagh and Nelder 1989; Dobson and Barnett 2008)
  - normal, Poisson, binomial/Bernoulli, multinomial, beta, gamma, lognormal, exponential, and Dirichlet
- Principles of linear modeling can be carried over to models other than normal linear regression 😎

see Chapter 3, Kery and Royle 2016

The Poisson GLM for unbounded counts

$$C_i \sim \text{Poisson}(\lambda_i)$$

$$\log(\lambda_i) = X_{i,j} \cdot \beta_{\mathbf{j}}$$

- C is count of observation i, $X_{i,j}$ is a design matrix, j is number of columns, β_j is a vector of parameters
- simulate Poisson data in R:

```r
set.seed(1)
rpois(n = 100, lambda = 15) # 100 deviates from lambda = 15
```

```
  [1] 12 20 19 16  9 16 17 17 13 20 16 12 13 13 15 11 18 17 18 18 15  7 16 19
12
 [26] 13 16 20 14 16 14  9 18 13 19 13 21 17 13 11 12  8 17 14 18 16 12 11 20
22
 [51] 13 10 10 24 14 17 15 12  9 20 15 23 16 12 14 17 19 15 14 11 12 19 17 14
13
```

The Poisson GLM for unbounded counts

$$C_i \sim \text{Poisson}(\lambda_i)$$

$$\log(\lambda_i) = X_{i,j} \cdot \beta_{\mathbf{j}}$$

- C is count of observation i, $X_{i,j}$ is a design matrix, j is number of columns, β_j is a vector of parameters
- log-probability mass of Poisson count data in R:

```
1 C_i <- c(10, 17, 18) # fake count data
2 dpois(x = C_i, lambda = 15, log = TRUE) # return log-Poisson likelihood
```

```
[1] -3.023911 -2.468220 -2.650542
```

The Poisson GLM for unbounded counts

$$C_i \sim \text{Poisson}(\lambda_i)$$

$$\log(\lambda_i) = X_{i,j} \cdot \beta_{\mathbf{j}}$$

- Assumptions
  - The mean and variance of the Poisson distribution are equal
  - Almost never holds and usually requires a negative binomial or another model structure
  - Causes of over/under dispersion are complex

see Chapter 3, Kery and Royle 2016; Zuur et al. 2017

Testing for over- or under-dispersion: Poisson GLM

- mean = variance = λ
- Another way: Bayesian p-value
- Idea: define a test statistic and compare the posterior distribution of that statistic for the original data to the posterior distribution of that test statistic for "replicate" datasets
- Note we could also use graphical posterior predictive checks

Gelman et al. 2006; see Chapter 3, Kery and Royle 2016; Zuur et al. 2017

Bayesian p-value

- Pearson residuals:

$$D\left(y_i, \theta\right) = \frac{\left(y_i - \mathrm{E}\left(y_i\right)\right)}{\sqrt{\mathrm{Var}(y_i)}}.$$

- Begin by calculating the sum of squared residuals (our test statistic) for the observed data:

$$T(\mathbf{y}, \theta) = \sum_i D(y_i, \theta)^2$$

Bayesian p-value

- Next, we calculate the same statistic for replicate (simulated) datasets

$$T\left(\mathbf{y}^{\text{new}}, \theta\right) = \sum_i D\left(y_i^{\text{new}}, \theta\right)^2$$

- Bayesian p-value is simply the posterior probability $\Pr(T\left(\mathbf{y}^{\text{new}}\right) > T(\mathbf{y}))$
- Should be close to 0.5 for a good model, too near 0 or 1 indicates lack of fit (somewhat subjective)

see Chapter 3, Kery and Royle 2016; Zuur et al. 2017

The binomial GLM for bounded counts or proportions

- Often have counts bounded by an upper limit
  - Number of successful breeding pairs cannot be higher than all observed breeding pairs
- Proportion of nestlings surviving
- These types of data require the binomial GLM

Kery and Schaub 2012

The binomial GLM for bounded counts or proportions

1. Random part of the response (statistical distribution)

$$C_i \sim \text{Binomial}(N_i, p_i)$$

2. Link of the random and systematic bit (logit link):

$$\text{logit}(p_i) = \log\left(\frac{p_i}{1 - p_i}\right) = \eta_i$$

3. Systematic part (linear predictor):

$$\eta_i = \beta_0 + \beta_1{}^* X_i + \beta_2{}^* X_i^2$$

The binomial GLM for bounded counts or proportions

$$C_i \sim \text{Binomial}(N_i, p_i)$$

$$\text{logit}(p_i) = \log\left(\frac{p_i}{1 - p_i}\right) = \eta_i$$

$$\eta_i = \beta_0 + \beta_1{}^* X_i + \beta_2{}^* X_i^2$$

- where p_i is expected proportion on arithmetic scale and is mean response of each of the observed N_i trials
- η_i is the same proportion but on the logit-link scale

The binomial GLM for bounded counts or proportions

$$\text{logit}(p_i) = \log\left(\frac{p_i}{1 - p_i}\right) = \eta_i$$

- Logit maps the probability scale (i.e., range 0 to 1) to the entire real line (i.e., -∞ to ∞)
- The rest of the model (linear predictor) is up to you, your data, your questions, and your imagination

Kery and Schaub 2012

Overdispersion and underdispersion in the binomial distribution

- Note that the binomial distribution variance is equal to

$$N \cdot p \cdot (1 - p)$$

- Need to check the binomial for under and over dispersion similar to how we check for the Poisson
- See this paper for some useful logistic regression checks

In-class exercise

In-class exercise

- Let's simulate a Poisson GLM, where we model peninsular homing clam 🥟 counts as a function of year:

$$C_i \sim \text{Poisson}(\lambda_i)$$

$$\log(\lambda_i) = \beta_0 + \beta_1 \cdot \text{year}_i + \beta_2 \cdot \text{year}_i^2 + \beta_3 \cdot \text{year}_i^3$$

- Clam counts follow a cubic polynomial function of time
  - Note this equation is still linear in the predictors
- Where do we begin?

Kery and Schaub 2012

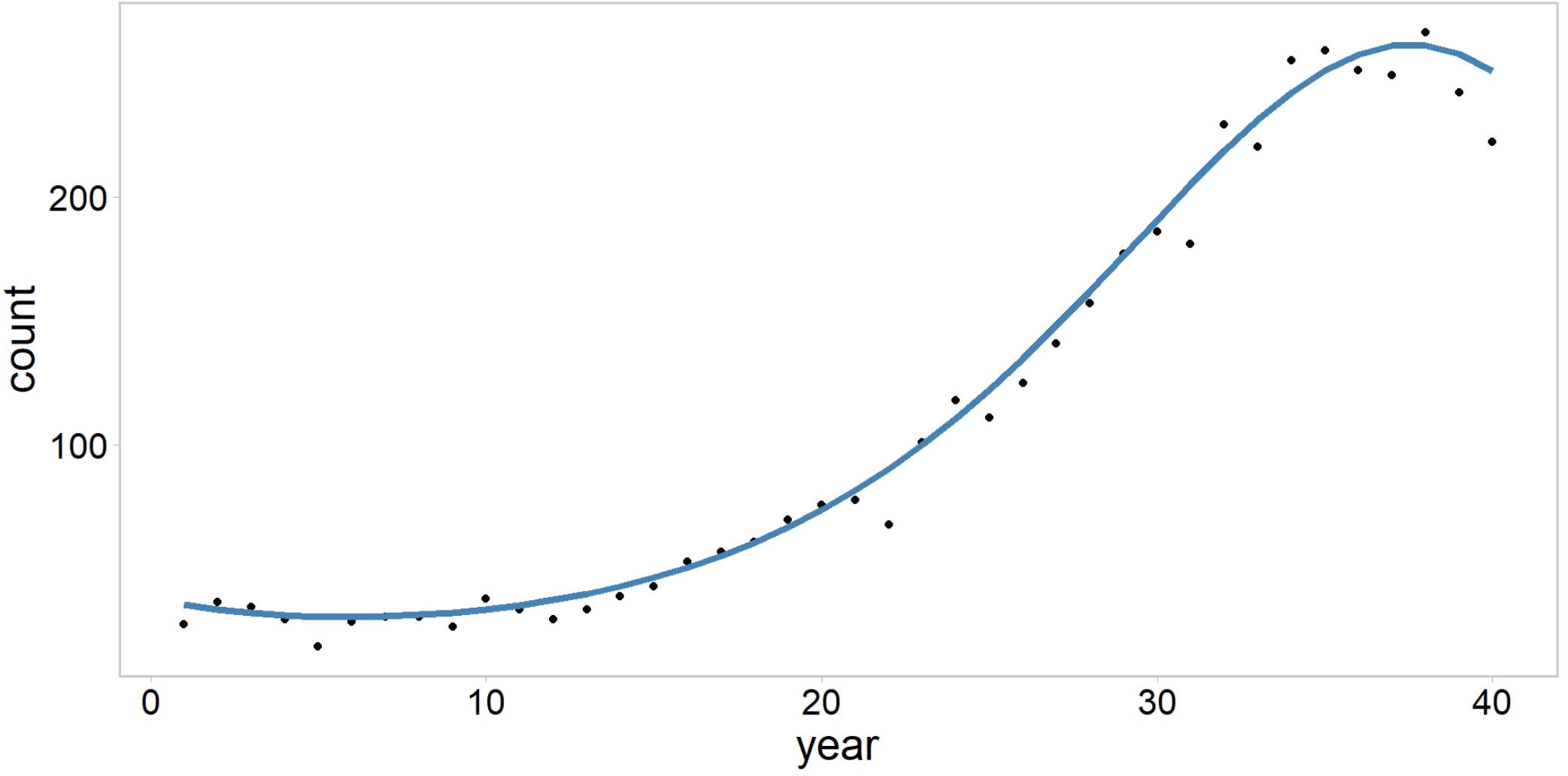
Peninsular homing clams 🫔: simulating fake data

- Let's get it started (in here)

```r
n_year <- 40
beta0 <- 3.5576
beta1 <-  -0.0912
beta2 <- 0.0091
beta3 <- -0.00014
set.seed(1)
```

- Exercise: see if you can generate fake data for this model
- Start by calculating the systematic component, then apply the link function, and lastly generate random deviates according to the Poisson distribution

Homing clam simulation solution



Coding the 🥟 model in Stan

- Assume Normal(0, 10) priors for everything
- Should look similar to the simulation code
- Hint: you will get a funny error message and we will work through it as a group

Writing the `clams.stan` file 

```
data {
  ...
}
parameters {
  ...
}
transformed parameters {
  ...
}
model {
  ...
}
```

- Work together to get this model estimating

Go to solution files

Summary and Recap

- We have covered much ground
- Statistical models as response = deterministic + random
  - ANCOVA
- Introduced GLMs, which allow us to model data coming from distributions other than the normal
- Examined Poisson and Binomial GLMs
- Talked about dispersion
- This material lays the critical groundwork for more complicated models

References

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