Generalized Additive Models!

Gavin Fay slides from Megan Winton (mwinton@umassd.edu) MAR 536 Biological Statistics II February 23 2023

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Generalized linear models: Quick review

Steps for fitting a GLM:

- I. Specify distribution for response variable
 - What we want to predict
- 2. Specify link function
 - Remember the link function calculates the expected value of the response variable given the linear predictor
- 3. Specify linear predictor

• What we think influences what we want to predict **Example:**

What is the relationship between counts of species *i* and covariate x?

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \mathbf{\beta} \mathbf{x}_i$

How do you choose which distribution?

Step I: Is your response variable DISCRETE or CONTINUOUS?

Common distributions for response variables

Step I: If DISCRETE

Name	Notation	Domain	Range
Bernoulli	$B \sim Bernoulli(p)$	$0 \le p \le 1$	B = {0, 1}
Binomial	N~Binomial(p,n)	$0 \le p \le 1$	N = {0, 1,, n}
Poisson	$N \sim Poisson(\lambda)$	λ>0	N = {0, 1,,∞}
Negative binomial	N~NegativeBinomial(λ,θ)	λ>0 θ>0	N = {0, 1,,∞}

Common distributions for response variables

Step I: If DISCRETE

Name	Notation	Domain	Range
Bernoulli	$B \sim Bernoulli(p)$	$0 \le p \le 1$	B = {0, 1}
Binomial	$N \sim Binomial(p, n)$	$0 \le p \le 1$	N = {0, 1,, n}
Poisson	$N \sim Poisson(\lambda)$	λ > 0	N = {0, 1,,∞}
Negative binomial	N~NegativeBinomial(λ,θ)	λ > 0 Θ > 0	N = {0, 1,,∞}

Step Ia: What is the range of possible values?

- 0 or I -> Bernoulli
- Between 0 and N (N is # of trials) -> Binomial
- >= 0 Poisson
- >= 0 and variance changes with mean -> Negative binomial

Common distributions for response variables

Step I: If CONTINUOUS

Name	Notation	Domain	Range
Normal	$Y \sim Normal(\mu, \sigma^2)$	$\sigma^2 > 0$	Unrestricted
Lognormal	$\log(Y) \sim Normal(\mu, \sigma^2)$	$\sigma^2 > 0$	Y > 0
Gamma	$Y \sim Gamma(\mu, CV)$	μ > 0 CV > 0	Y > 0
Beta	$p \sim Beta(\alpha, \beta)$	$\alpha > 0, \beta > 0$	0 < p < 1

Step 1b: What is the range of possible values?

- -∞ to +∞ -> Normal
- > 0 -> Lognormal or Gamma
- > 0 and < I -> Beta

Step 1b: Is there precedent?

Choice of link functions

Step 2: Specify link function based on selected distribution

 Remember that the link function acts like transformation of the

response variable.

- The link function establishes the connection between the linear predictor and the mean of the distribution.
- There is a 'natural link' associated with each distribution the canonical link function
 - For our Poisson example:

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta \mathbf{x}_i$

- Canonical link is typically used, but don't neglect alternatives
 - Enter ?family to see options in R

What makes GLMs linear?

Step 3: Specify linear predictor

- Linear predictor expresses our hypothesis about what influences our response variable
- In a GLM, all terms in the linear predictor are linear.
 - Expanding on our Poisson example:

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta_0 + \beta_1 \text{Time}_i + \beta_2 \text{Temp}_i$

What makes GLMs linear?

Step 3: Specify linear predictor

- Linear predictor expresses our hypothesis about what influences our response variable
- In a GLM, all terms in the linear predictor are linear.
 - Expanding on our Poisson example:

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta_0 + \beta_1 \text{Time}_i + \beta_2 \text{Temp}_i$

• If we suspect things are nonlinear, we can include a polynomial: $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta_0 + \beta_1 \text{Time}_i + \beta_2 \text{Temp}_i + \beta_3 \text{Temp}_i^2$

What makes GLMs linear?

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 - Expanding on our Poisson example:

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta_0 + \beta_1 \text{Time}_i + \beta_2 \text{Temp}_i$

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This is still a GLM!

Getting to GAMs

Step 3: Specify linear predictor

- A GAM includes at least one nonlinear smoothing function or spline.
- To make our Poisson example a GAM:

$$c_i \sim Poisson(\lambda_i)$$

$$\log(\lambda_i) = \beta_0 + \beta_1 \text{Time}_i + f(\text{Temp}_i)$$

- Always use 'mgcv' rather than default gam()!
- There are tons of splines to choose from.

** A 'regular' additive model is just a GAM assuming a normal distribution with an identity link function.

Spline types in package 'mgcv'

Thin plate spline (tp):

- does not use knots
- can be used for multiple covariates (i.e., for interactions)
- computationally expensive

Cubic regression splines (cr):

- uses knots
- can only be used for single covariates
- computationally less expensive

Cyclic cubic regression splines (cc):

- A cr, but has the same start and end point (e.g. for modelling seasonality)

Spline types in package 'mgcv'

Splines with shrinkage: allow for the complete removal of covariates during fitting if they are not needed

- Thin plate spline with shrinkage (ts):
- Cubic regression splines with shrinkage (cs):

Tensor products (te):

- another alternative if you have multiple covariates with interactions
- Advantage = invariant to relative scaling of covariates
- And more!
 - Enter ?smooth.terms after loading the 'mgcv' library in R

Motivating example

Can we identify seasonal trends in yellowtail flounder bycatch in the sea scallop fishery to inform bycatch mitigation measures?



Motivating example

Coonamessett Farm Foundation's seasonal bycatch survey



Simplest possible model

What is the mean catch of YT per survey tow?

of YT per 30 minute tow

Remember our GLM fitting steps!

- I. Specify distribution for response variable
- 2. Specify link function
- 3. Specify linear predictor

Simplest possible model

What is the mean catch of YT per survey tow?

of YT per 30 minute tow

Remember our GLM fitting steps!

- I. Specify distribution for response variable
 - Counts -> Poisson:

 $c_i \sim Poisson(\lambda_i)$

- 2. Specify link function
 - We'll go with the canonical link function -> log link
 - (? family in R for others)
- 3. Specify linear predictor
 - Intercept only

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta_0$

Fitting in R

Using the glm() command:

> glm0 = glm(catch~1,data=dat2,family=poisson(link="log"))

```
> summary(g1m0)
Call:
glm(formula = catch \sim 1, family = poisson(link = "log"), data = dat2)
Deviance Residuals:
    Min
             10 Median
                               30
                                       Max
-3.7625 -2.8709 -1.2612 0.6929 24.2451
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) 1.95702 0.01284 152.4 <2e-16 ***
____
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for poisson family taken to be 1)
    Null deviance: 8485.4 on 856 degrees of freedom
Residual deviance: 8485.4 on 856 degrees of freedom
AIC: 10983
Number of Fisher Scoring iterations: 6
> \exp(1.957)
[1] 7.078061
> summary(dat2$catch)
   Min. 1st Qu.
                Median
                        Mean 3rd Qu.
                                          Max.
  0.000 1.000
                4.000 7.078 9.000 143.000
```

Our model:

```
c_i \sim Poisson(\lambda_i)\log(\lambda_i) = \beta_0
```

Fitting in R

Using the gam() command in package 'mgcv':

> m0 = gam(catch~1,data=dat2,family=poisson(link="log"))

```
> summary(m0)
Family: poisson
Link function: log
Formula:
catch \sim 1
Parametric coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) 1.95702 0.01284 152.4 <2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R-sq.(adj) = 0 Deviance explained = -2.14e-13%
UBRE = 8.9036 Scale est. = 1 n = 857
>
```

That was pretty boring...

There are very few situations where an intercept-only model will be informative (except as a baseline for model selection).



Histogram of YT catch

Number of yellowtail flounder per tow

Specifying the linear predictor

We might expect that bycatch rates vary seasonally due to YT movements or factors impacting their response time (e.g. water temperature).



YT catch by month

Month

Specifying the linear predictor

A logical first step might be to include month as a factor (i.e. a categorical variable).

> m1 = gam(catch~as.factor(Month),data=dat2,family=poisson(link="log"))

> summary(m1)

Family: poisson Link function: log

Formula: catch ~ as.factor(Month)

Parametric coefficients:

	Estimate	Std. Error	z value	Pr(> z)	
(Intercept)	1.763268	0.043895	40.170	< 2e-16	***
as.factor(Month)2	0.133852	0.083227	1.608	0.107775	
as.factor(Month)3	-0.290487	0.062077	-4.679	2.88e-06	***
as.factor(Month)4	-0.008156	0.062381	-0.131	0.895974	
as.factor(Month)5	-0.284858	0.076986	-3.700	0.000215	***
as.factor(Month)6	-0.679581	0.075407	-9.012	< 2e-16	***
as.factor(Month)7	-0.259190	0.075037	-3.454	0.000552	***
as.factor(Month)8	0.774320	0.057565	13.451	< 2e-16	***
as.factor(Month)9	0.994294	0.051456	19.323	< 2e-16	***
as.factor(Month)10	0.749496	0.057449	13.046	< 2e-16	***
as.factor(Month)11	0.661535	0.069833	9.473	< 2e-16	***
as.factor(Month)12	-0.382544	0.068703	-5.568	2.58e-08	***
Signif. codes: 0	'***' 0.001	L'**' 0.01	'*' 0.0	5 '.' 0.1	''1
-					
R-sq.(adj) = 0.145 Deviance explained = 22.3%					
UBRE = 6.7241 Sca	le est. = 1	L n	= 857		
>					

Our model is now:

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta_0 + \beta_{i,Monthi}$

Interpretation of results

A logical first step might be to include month as a factor (i.e. a categorical variable).

> m1 = gam(catch~as.factor(Month),data=dat2,family=poisson(link="log"))

> summary(m1)

Family: poisson Link function: log

Formula: catch ~ as.factor(Month)

Parametric coefficients:

	Estimate	Std. Error	z value	Pr(> z)	
(Intercept)	1.763268	0.043895	40.170	< 2e-16	***
as.factor(Month)2	0.133852	0.083227	1.608	0.107775	
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as.factor(Month)7	-0.259190	0.075037	-3.454	0.000552	***
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as.factor(Month)10	0.749496	0.057449	13.046	< 2e-16	***
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R-sq.(adj) = 0.145 Deviance explained = 22.3%					
UBRE = 6.7241 Scale est. = 1 n = 857					
>					

Interpretation:

- To predict value in each month, add coefficient to the intercept
 - Intercept corresponds to January
- Explained more of the observed variation than the intercept-only model.

Interpretation of results

A logical first step might be to include month as a factor (i.e. a categorical variable).

> m1 = gam(catch~as.factor(Month),data=dat2,family=poisson(link="log"))

> summary(m1)

Family: poisson Link function: log

Formula: 140 0 catch \sim as.factor(Month) 120 Parametric coefficients: Estimate Std. Error z value Pr(>|z|)(Intercept) 1.763268 0.043895 40.170 < 2e-16 *** 100 Number of YT caught as.factor(Month)2 0.133852 0.083227 1.608 0.107775 0 as.factor(Month)3 -0.290487 0.062077 -4.679 2.88e-06 *** 8 as.factor(Month)4 -0.008156 0.062381 -0.131 0.895974 0 as.factor(Month)5 -0.284858 0.076986 -3.700 0.000215 *** 0 as.factor(Month)6 -0.679581 0.075407 - 9.012 < 2e - 16 $\star \star \star$ 8 0 as.factor(Month)7 -0.259190 0.075037 - 3.454 0.000552*** 0 as.factor(Month)8 0.774320 0.057565 13.451 < 2e-16 *** 0 as.factor(Month)9 0.994294 0.051456 19.323 < 2e-16 *** 4 as.factor(Month)10 0.749496 0.057449 13.046 < 2e-16 *** 8 as.factor(Month)11 0.661535 0.069833 9.473 < 2e-16 *** 8 as.factor(Month)12 -0.382544 0.068703 -5.568 2.58e-08 *** Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 0 2 12 З 5 6 g 10 11 Deviance explained = 22.3%R-sq.(adj) = 0.145UBRE = 6.7241 Scale est. = 1 n = 857Month 5

YT catch by month

Specifying a continuous, linear seasonal effect

Based on the boxplot, it might make sense to model YT catch as a linear function of month.

> m2 = gam(catch~Month,data=dat2,family=poisson(link="log"))

```
> summary(m2)
                                                 Our model is
Family: poisson
                                                 now:
Link function: log
                                                 c_i \sim Poisson(\lambda_i)
Formula:
catch \sim Month
                                                  \log(\lambda_i) = \beta_0 + \beta_1 \operatorname{Month}_i
Parametric coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) 1.504082 0.029246 51.43 <2e-16 ***
           0.068112 0.003724 18.29 <2e-16 ***
Month
___
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R-sq.(adj) = 0.0211 Deviance explained = 3.96%
UBRE = 8.514 Scale est. = 1 n = 857
>
```

YT catch by month



Month

2

Zoomed in (and not plotting points for tows):

4

Number of YT per tow

6

Month

8

10

12

YT catch by month

Not surprisingly, residual plot doesn't look great, either:



Month

What do we do when things aren't linear?

Fit a polynomial: Many animals exhibit seasonal cycles – maybe a 3rd order polynomial will do?

> m3 = gam(catch~poly(Month,3),data=dat2,family=poisson(link="log"))

```
> summary(m3)
                                     Our model is now:
Family: poisson
                                            c_i \sim Poisson(\lambda_i)
Link function: log
                         \log(\lambda_i) = \beta_0 + \beta_1 \text{Month}_i + \beta_2 \text{Month}_i^2 + \beta_3 \text{Month}_i^3
Formula:
catch ~ poly(Month, 3)
Parametric coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept) 1.84683
                             0.01424 129.688 < 2e-16 ***
poly(Month, 3)1 6.74500 0.39915 16.899 < 2e-16 ***
poly(Month, 3)2 -1.78638 0.39403 -4.534 5.8e-06 ***
poly(Month, 3)3 -11.75134 0.39744 -29.568 < 2e-16 ***
_ _ _
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R-sq.(adj) = 0.116 Deviance explained = 15.5%
UBRE = 7.3736 Scale est. = 1 n = 857
>
```

YT catch by month



Month

What if the nonlinear relationship is more complex?

Fit a generalized additive model: s() notation

> m4 = gam(catch~s(Month),data=dat2,family=poisson(link="log"))

```
> summary(m4)
```

Our model is now:

```
Family: poisson
Link function: log
```

```
Formula:
catch ~ s(Month)
```

```
c_i \sim Poisson(\lambda_i)
\log(\lambda_i) = \beta_0 + f(Month_i)
```

gam() optimizes smoothness selection for you

• Automatically determines the degrees of freedom for every section of the smoothing function

$$CV(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \left(\left(Y_i - \widehat{f_{\lambda}^{-i}}(X_i) \right) \right)^2$$

* The -i means the ith observation was removed & λ is the amount of smoothing

- GCV is generalized cross validation & is a modified version of cross validation that finds an optimal parameter value based on cross validation.
- A GCV (or UBRE) score will be included in the output
 - The lower the value, the better the fit (similar to AIC).
- Can also fit via maximum likelihood by specifying method="ML" (recommended)

gam() optimizes smoothness selection for you



Interpreting gam() output

Fit a generalized additive model: s() notation

```
> m4 = gam(catch~s(Month), data=dat2, family=poisson(link="log"))

> summary(m4)

Family: poisson

Link function: log

Formula:

Our model is now:

c_i \sim Poisson(\lambda_i)

\log(\lambda_i) = \beta_0 + f(Month_i)
```

```
Formula:
catch ~ s(Month)
```

>

Interpreting gam() output

Fit a generalized additive model: s() notation

```
> m4 = gam(catch~s(Month), data=dat2, family=poisson(link="log"))

> summary(m4)

Family: poisson

Link function: log

Formula:

Our model is now:

c_i \sim Poisson(\lambda_i)

\log(\lambda_i) = \beta_0 + f(Month_i)
```

```
Formula:
catch ~ s(Month)
```



Month

Spline selection: you've got options!

Fit a generalized additive model: s(, bs =) notation

> m5 = gam(catch~s(Month,bs='cc'),data=dat2,family=poisson(link="log"))

```
> summary(m3)
                                                  Our model is now:
Family: poisson
                                                      c_i \sim Poisson(\lambda_i)
Link function: log
                                                   \log(\lambda_i) = \beta_0 + f(Month_i)
Formula:
catch ~ Month + I(Month^2)
Parametric coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) 1.129041 0.054723 20.632 <2e-16 ***
      0.212075 0.017542 12.090 <2e-16 ***
Month
I(Month^2) -0.010490 0.001243 -8.439 <2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R-sq.(adj) = 0.0332 Deviance explained = 4.82%
UBRE = 8.4306 Scale est. = 1 n = 857
>
```

Spline selection: you've got options!

Fit a generalized additive model: s(, bs =) notation

> m5 = gam(catch~s(Month,bs='cc'),data=dat2,family=poisson(link="log"))

```
> summary(m5)
Family: poisson
Link function: loa
Formula:
catch \sim s(Month, bs = "cc")
Parametric coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) 1.81270 0.01463 123.9 <2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Approximate significance of smooth terms:
          edf Ref.df Chi.sg p-value
s(Month) 7.892
                   8 1837 <2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R-sq.(adj) = 0.145 Deviance explained = 21.6%
UBRE = 6.7843 Scale est. = 1 n = 857
>
```

Our model is still:

```
c_i \sim Poisson(\lambda_i)
\log(\lambda_i) = \beta_0 + f(Month_i)
```



Month

Including interaction terms in a smoother

Fit a generalized additive model: s(, by =) notation

> m6 = gam(catch~s(Month,by=Lat),data=dat2,family=poisson(link="log"))

> summary(m6)

Our model is now:

Family: poisson Link function: log

```
Formula:
catch ~ s(Month, by = as.factor(latitude))
```

 $c_i \sim Poisson(\lambda_i)$ $\log(\lambda_i) = \beta_0 + f(Month_i * Latitudei)$



Model selection and validation

How do we assess fit?

Significance testing (not my favorite):

- Add or remove explanatory variables based on F- or likelihood ratio tests
 - Do not use default R output p-values!
- Information theoretic approaches
 - Measure predictive 'loss'
 - Akaike Information Criteria (AIC)
 - Need to be careful with edf the debate rages on
- Best approach (for now):
 - Selection via AIC backed up with cross validation
- Model validation
 - Inspect residual and other diagnostic plots carefully

> /	AIC(m0,m1,m	n2,m3,m4,m5,m6)
	df	AIC
mO	1.000000	10983.282
m1	12.000000	9115.437
m2	2.000000	10649.363
m3	4.000000	9672.105
m4	9.864632	9126.083
m5	8.891544	9166.999
m6	42.645039	8538.063

Is all this wiggliness a good idea?



Words of caution

You may be tempted to use GAMs for everything (GAMania)

- Tendency to overfit data (i.e., be too wiggly), even when using penalized splines
 - Can limit predictive usefulness
- A lot of times, a well formulated polynomial can do almost as good of a job fitting to the data
 - Have more informative parameter estimates/greater
 predictive power
- Importance of model validation
 - Inspect residual and other diagnostic plots carefully
 - If we had time to do this, we would have discovered a lot of problems with our YT model.
- Use your biological intuition!

Coming back to our YT example



Extensions

Spatial models



Extensions

Spatiotemporal models – when response varies over space and time



Zero-inflated models – when response contains many zeros

• Probably appropriate for our YT example

Mixed effects models/hierarchical models – incredibly useful

- When observations are correlated
- Or when you are interested in a phenomena that is not directly observable, but can be inferred from your data

Useful References

Hastie, T.J. and R.J. Tibshirani. 1990. Generalized Additive Models.: Chapman and Hall. New York.

Venables, W. N. and C. M. Dichmont. 2004. GLMs, GAMs and GLMMs: an overview of theory for applications in fisheries research. Fisheries Research, 2004.

Wood, S.N., 2006. Generalized Additive Models: An Introduction with R. Chapman & Hall, London.

Zuur, A. et al. 2009. Mixed Effects Models and Extensions in Ecology with R. Springer-Verlag New York.



2/28: Matrix Algebra Review

3/01: Lab 7 (writing your own functions)

3/02: Principal Components Analysis