

Modeling Non-linear relationships

FW8051 Statistics for Ecologists

Department of Fisheries, Wildlife and Conservation Biology



Learning objectives:

- Be able to implement common approaches for modeling non-linear relationships between X_i and Y_i
 - Polynomials using the `poly` function in R
 - Splines using the `ns` function (splines library)
 - Smoothing splines
- Understand how model predictions are constructed when using polynomials or splines

Mallard clutch size versus Julian Date

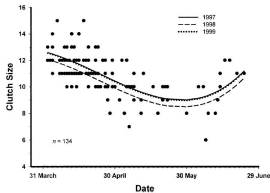
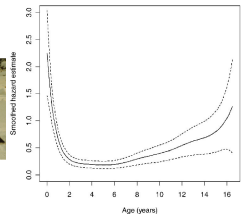
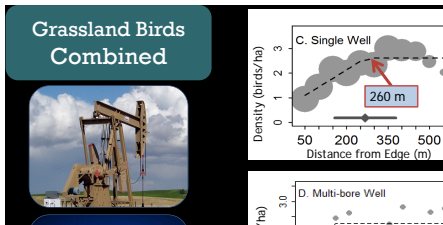


FIG. 2. Mallard clutch size in nest structures was modeled as having a curvilinear relationship to nest initiation date in western Minnesota, 1997–1999.



Age-specific Hazard for White-tailed Deer





So far, we have focused on *linear models* of the form:

$$Y_i = \beta_0 + X_i \beta + \epsilon_i$$

or

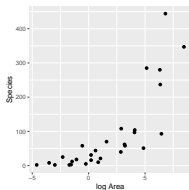
$$Y_i = \beta_0 + X_{i,1} \beta_1 + X_{i,2} \beta_2 + \dots + \epsilon_i$$

The model can be written as a "linear combination" of parameters.

Species-Area relationship

Plant species richness for 29 islands in the Galapagos Islands archipelago (Johnson and Raven 1973)¹

```
ggplot(gala, aes(x=logarea, y=Species)) + geom_point(size=3) +  
  xlab("log Area") + theme_gray(base_size=20)
```



Modeling Non-Linear Relationships

- Polynomials (e.g., $\text{poly}(\text{age}, 2)$ for a quadratic in age)
- Transformations of X or Y (e.g., $\log(X)$, \sqrt{Y} , $\exp(X)$).
- Regression splines

These options still lead to *linear models*:

$$Y_i = \beta_0 + X_i \beta_1 + X_i^2 \beta_2 + \dots + \epsilon_i$$

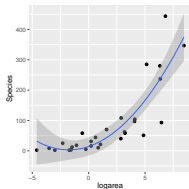
$$\sqrt{Y_i} = \beta_0 + \log(X_i) \beta_1 + \dots + \epsilon_i$$

So, we can use all the same tools we've learned about (e.g., residual plots, t-tests, F-tests, AIC, etc) [note: try writing out the above models in matrix notation!]

¹<http://www.ibiblio.org/pub/academic/biology/ecology+evolution/teaching/weisberg>

Species-Area relationship

```
ggplot(gala, aes(x=logarea, y=Species)) + geom_point(size=3) +  
  geom_smooth(method="lm", formula=y~poly(x,2), se=TRUE) +  
  theme_grey(base_size=20)
```



Polynomials

```
gala$logarea.squared<-gala$logarea^2  
lm.poly<-lm(Species~ logarea + logarea.squared, data=gala)  
summary(lm.poly)
```

```
Call:  
lm(formula = Species ~ logarea + logarea.squared, data = gala)
```

```
Residuals:  
    Min       1Q   Median       3Q      Max  
-151.009  -27.361   -1.033   20.825   178.805
```

```
Coefficients:  
              Estimate Std. Error t value Pr(>|t|)  
(Intercept)   14.1530    14.5607   0.972  0.340010  
logarea        12.6226     4.8614   2.596  0.015293 +  
logarea.squared 3.5641     0.9445   3.773  0.000842 ***  
---  
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Residual standard error: 59.88 on 26 degrees of freedom  
Multiple R-squared:  0.7528,    Adjusted R-squared:  0.7338  
F-statistic: 39.6 on 2 and 26 DF,  p-value: 1.285e-08
```

Polynomials

```
lm.poly1.raw<-lm(Species~ poly(logarea,2, raw=TRUE), data=gala)  
summary(lm.poly1.raw)
```

```
Call:  
lm(formula = Species ~ poly(logarea, 2, raw = TRUE), data = gala)
```

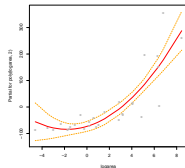
```
Residuals:  
    Min       1Q   Median       3Q      Max  
-151.009  -27.361   -1.033   20.825   178.805
```

```
Coefficients:  
              Estimate Std. Error t value Pr(>|t|)  
(Intercept)   14.1530    14.5607   0.972  0.340010  
poly(logarea, 2, raw = TRUE)1  12.6226     4.8614   2.596  0.015293 +  
poly(logarea, 2, raw = TRUE)2   3.5641     0.9445   3.773  0.000842 ***  
---  
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Residual standard error: 59.88 on 26 degrees of freedom  
Multiple R-squared:  0.7528,    Adjusted R-squared:  0.7338  
F-statistic: 39.6 on 2 and 26 DF,  p-value: 1.285e-08
```

Polynomials: component + residual plot

```
lm.poly1.raw<-lm(Species~ poly(logarea,2), data=gala)  
termplot(lm.poly1.raw, se=T, partial=T, pch=16)
```



Hypothesis Testing

```
library(car)
Anova(lm.poly) #log(Area)+ I(log(Area)^2)
```

Anova Table (Type II tests)

Response: Species

	Sum Sq	Df	F value	Pr(>F)
logarea	24175	1	6.7417	0.0152925 *
logarea.squared	51058	1	14.2387	0.0008418 ***
Residuals	93232	26		

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```
Anova(lm.poly1.raw) # poly(logarea,2)
```

Anova Table (Type II tests)

Response: Species

	Sum Sq	Df	F value	Pr(>F)
poly(logarea, 2)	283970	2	39.596	1.285e-08 ***
Residuals	93232	26		

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```
head(model.matrix(Species~ poly(logarea,2, raw=TRUE), data=gala))
```

	(Intercept)	poly(logarea, 2, raw = TRUE)1	poly(logarea, 2, raw = TRUE)2
1	1	3.2224694	10.38430878
2	1	0.2151114	0.04627291
3	1	-1.5606477	2.43562139
4	1	-2.3025851	5.30189811
5	1	-2.9957323	8.97441185
6	1	-1.0788097	1.16383029

Basis functions/vectors

A *linear model* is a model that is linear in the parameters:

$$Y_i = \sum_{j=1}^P \beta_j b_j(X_i) + \epsilon_i$$

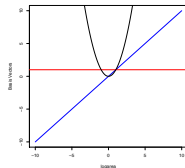
The $b_j(X_i)$ are called **basis functions** or **basis vectors**.

$$Y_i = \beta_0 + \beta_2 X_i + \beta_3 X_i^2 + \dots + \epsilon_i$$

$$b_j(X_i) = 1, X, X^2, X^3, \dots$$

Basis functions

$$E[Y_i|X_i] = \beta_0 1 + \beta_2 X_i + \beta_3 X_i^2$$

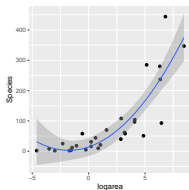


$E[Y|X]$ is given by a linear combination of a horizontal line (1), a line through the origin (X), a quadratic centered on the origin (X^2), etc.

Species-Area relationship

$$\text{Species}_i = 14.15 + 12.62X_i + 3.56X_i^2$$

```
ggplot(gala, aes(x=logarea, y=Species)) + geom_point(size=3) +
  geom_smooth(method="lm", formula=y~poly(x,2, raw=TRUE)) +
  theme_grey(base_size=20)
```



Polynomials

A **polynomial of degree D** is a function formed by linear combinations of the powers of its argument up to D:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots + \beta_D x^D$$

Specific polynomials:

Linear $y = \beta_0 + \beta_1 x$

Quadratic $y = \beta_0 + \beta_1 x + \beta_2 x^2$

Cubic $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$

Quartic $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4$

Quintic $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \beta_5 x^5$

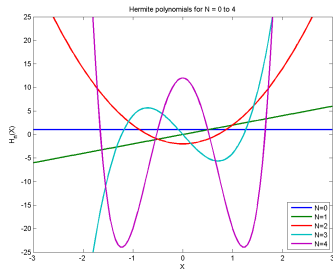
Polynomials

The **design matrix** for a regression model with n observations and p predictors is the matrix with n rows and p columns such that the value of the j^{th} predictor for the i^{th} observation is located in column j of row i .

Design matrix for a polynomial of degree D

$$\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \dots & x_1^D \\ 1 & x_2 & x_2^2 & x_2^3 & \dots & x_2^D \\ 1 & x_3 & x_3^2 & x_3^3 & \dots & x_3^D \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & \dots & x_n^D \end{bmatrix}$$

Polynomials



Orthogonal Polynomials

Standard polynomials can cause numerical issues due to differences in scale:

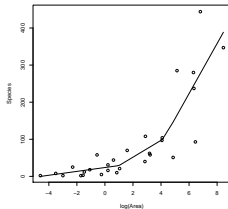
$$X = 100 x^3 = 1,000,000$$

Centering and scaling X can help.

Alternatively, we can use 'orthogonal polynomials' created using `poly(raw=FALSE)` (the default). See Section 4.10 in the book.

Species-Area relationship

Linear models are often a good approximation over small ranges of x .



Splines

Splines are piecewise polynomials used in curve fitting.

A **linear spline** is a continuous function formed by connecting linear segments. The points where the segments connect are called the **knots** of the spline.

Linear spline with knots at 1 and 4.2

```
gala$logarea<- log(gala$Area)
gala$logarea.1<- ifelse(gala$logarea<1, 0, gala$logarea-1)
gala$logarea.4.2<- ifelse(gala$logarea<4.2, 0, gala$logarea-4.2)
lm.sp<-lm(Species~logarea+logarea.1+logarea.4.2, data=gala)
summary(lm.sp)
```

Call:

```
lm(formula = Species ~ logarea + logarea.1 + logarea.4.2, data = gala)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-160.691	-16.547	-4.209	13.133	166.430

Coefficients:

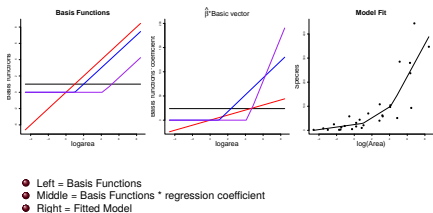
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	23.869	17.384	1.373	0.1819
logarea	5.213	8.956	0.582	0.5658
logarea.1	17.464	18.836	0.927	0.3627
logarea.4.2	44.815	23.156	1.935	0.0643

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 58.97 on 25 degrees of freedom

Multiple R-squared: 0.7695, Adjusted R-squared: 0.7418

Basis functions



Splines

A **spline of degree D** is a function formed by connecting polynomial segments of degree D so that:

- the function is continuous (no 'jumps')
- the function has D-1 continuous derivatives
- the D^{th} derivative is constant between knots

Linear splines (D = 1): first derivative is not constant (can go from increasing to decreasing at a knot)

Cubic Regression Splines

- Fits a cubic polynomial on segments of the data
- D-1 = 2 continuous derivatives everywhere (even at the knot locations)
 - the first derivative (tells us if the function is increasing or decreasing) is continuous (even at the knots)
 - the second derivative (tell us about curvature) is constant (even at the knots)
- Ensures that the fit is "smooth" at the connections (knot locations)

Simple Splines: Truncated Power Basis

The **truncated polynomial** of degree D associated with a knot ξ_k is the function which is equal to 0 to the left of ξ_k and equal to $(x - \xi_k)^D$ to the right of ξ_k .

$$(x - \xi_k)_+^D = \begin{cases} 0 & \text{if } x < \xi_k \\ (x - \xi_k)^D & \text{if } x \geq \xi_k \end{cases}$$

The equation for a spline of degree D with K knots is:

$$y = \beta_0 + \sum_{d=1}^D \beta_D x^d + \sum_{k=1}^K b_k (x - \xi_k)_+^D$$

Splines

The design matrix for a cubic spline with K knots is the n by $1 + 3 + K$ matrix with entries:

$$\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & (x_1 - \xi_1)_+^3 & \dots & (x_1 - \xi_K)_+^3 \\ 1 & x_2 & x_2^2 & x_2^3 & (x_2 - \xi_1)_+^3 & \dots & (x_2 - \xi_K)_+^3 \\ 1 & x_3 & x_3^2 & x_3^3 & (x_3 - \xi_1)_+^3 & \dots & (x_3 - \xi_K)_+^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & (x_n - \xi_1)_+^3 & \dots & (x_n - \xi_K)_+^3 \end{bmatrix}$$

Span: Splines

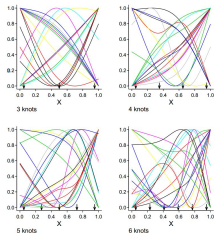


Figure 2.8: Some typical restricted cubic spline functions for $k = 3, 4, 5, 6$. The y-axis is X^3 . Arrows indicate knots. These curves were derived by randomly choosing values of β subject to standard deviations of fitted functions being normalized.

Basis functions: Splines

Truncated power basis:

- Easiest to understand, but may run into numerical problems due to scaling issues

Bsplines (`bs(x, df=)` in `splines` package)

- Numerically more stable than those based on the truncated power basis
- Can be poorly behaved in the tails

Natural or restricted cubic splines (`ns(x, df=)` in `splines` package; `rCs(x, df)` in `rCs` package)

- Fit is constrained to be linear before the first knot and after the last knot (these are referred to as *boundary knots*)
- Requires fewer model df (number of knots - 1 = number of interior knots + 1)

Natural Splines

```
lm.ns <- lm(Species ~ ns(logarea, df=3), data=gala)
summary(lm.ns)
```

Call:

```
lm(formula = Species ~ ns(logarea, df = 3), data = gala)
```

Residuals:

Min	1Q	Median	3Q	Max
-156.173	-13.819	-5.998	13.922	170.555

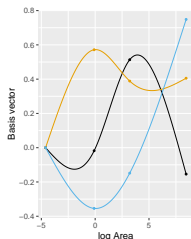
Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	1.468	43.542	0.034	0.9734
ns(logarea, df = 3)1	47.790	45.957	1.040	0.3084
ns(logarea, df = 3)2	276.125	102.146	2.703	0.0122 *
ns(logarea, df = 3)3	381.743	45.084	8.467	8.22e-09 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 59.48 on 25 degrees of freedom
Multiple R-squared: 0.7655, Adjusted R-squared: 0.7374
F-statistic: 27.21 on 3 and 25 DF, p-value: 4.859e-08

Natural Splines: Basis Vectors



Spline
 S1
 S2
 S3

```
attr(,"ns(gala$logarea,3)", "knots")
      33.33333%  66.66667%
-0.09393711  3.20877345

attr(,"ns(gala$logarea,3)", "Boundary.knots")

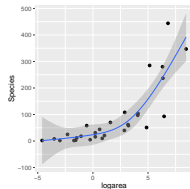
[1] -4.605170  8.448769

range(gala$logarea)

[1] -4.605170  8.448769
```

Natural Splines

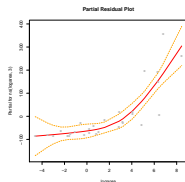
```
ggplot(gala, aes(x=logarea, y=Species)) + geom_point(size=3) +
  geom_smooth(method="lm", formula=y~ns(x,3), se=TRUE) +
  theme_grey(base_size=20)
```



Natural Splines

Compare fit to that of linear model

```
termplot(lm.ns, se=T, partial=T, pch=16, main="Partial Residual Plot")
```



```
lmfit<-lm(Species~ logarea, data=gala)
AIC(lmfit, lm.poly1.raw, lm.sp, lm.ns)
```

	df	AIC
lmfit	3	335.1547
lm.poly1.raw	4	324.4895
lm.sp	5	324.4646
lm.ns	5	324.9600

Any and all approaches fit better than a linear model!

Number of knots and their locations

The shape of a spline can be controlled by carefully choosing the number of knots and their exact locations in order to:

- Allow flexibility where the trend changes quickly, and
- Avoid overfitting where the trend changes little.

Could in principle compare models (e.g., using AIC) that have varying numbers of knots, or different knot locations

- Danger of overfitting, and difficult to account for model-selection uncertainty

Number of knots and their locations

Choose a small number of knots (df), based on how much data you have and how complex you expect the relationship to be *a priori*

- I've found that 2 or 3 internal knots are usually sufficient for small data sets
- Keele (2008), cited in Zuur et al, recommend 3 knots if $n < 30$ and 5 knots if $n > 100$

Choose knot locations based on quantiles (what `ns` does by default if you do not provide knot locations)

- Models fit with *cubic* regression splines are *usually* not too sensitive to knot locations

Knots

```
attr(,"ns(gala$logarea,3)", "knots")
```

```
33.33333% 66.66667%  
-0.09393711 3.20877345
```

```
attr(,"ns(gala$logarea,3)", "Boundary.knots")
```

```
[1] -4.605170 8.448769
```

```
range(gala$logarea)
```

```
[1] -4.605170 8.448769
```

Generalized Additive Models

See Section 4.7 of the book.

$$E[Y|X] = \beta_0 + f(x_1)$$

where $f(x_1)$ can be modeled in a variety of ways

- Smoothing splines
- Loess (locally weighted linear regression)

Smoothing or Penalized Splines

Smoothing splines:

Use lots of knots, but then attempt to balance overfitting and smoothness.

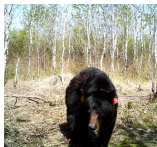
This balance can be accomplished by controlling the **size** of the spline coefficients (which reflect changes in the function over different portions of the data range).

Other considerations

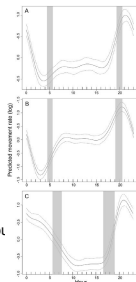
What if you want to allow for multiple non-linear relationships?

- $ns(x1, 3) + ns(x2, 4)$ or multiple smoothing splines
- Other basis functions can be used to fit 'smooth surfaces' (allowing for interactions between variables)
 - tensor splines, thin plate splines, etc. . .
- Can include interactions (separate smooth for each level of a categorical variable)

Black Bear Movement and Heart Rates



There are cyclical splines that ensure ends meet at 0 and 24 hours (or, Jan 1 and Dec 31).



Non-Linear Models with Mechanistic Basis

$Y \sim f(x, \beta)$, where $f(x, \beta)$ may have a strong theoretical motivation.

- Ricker model for stock-recruitment: $S_{t+1} = S_t e^{(1-\beta S_t)}$
- Predator prey: $f(N) = \frac{aN}{1+ahN}$

We will eventually learn how to fit these models using Maximum likelihood and Bayesian methods.