Modeling Non-linear relationships

FW8051 Statistics for Ecologists

Department of Fisheries, Wildlife and Conservation Biology

Modeling Non-linear relationships

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

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  - Smoothing splines
- Understand how model predictions are constructed when using polynomials or splines

Mallard clutch size versus Julian Date

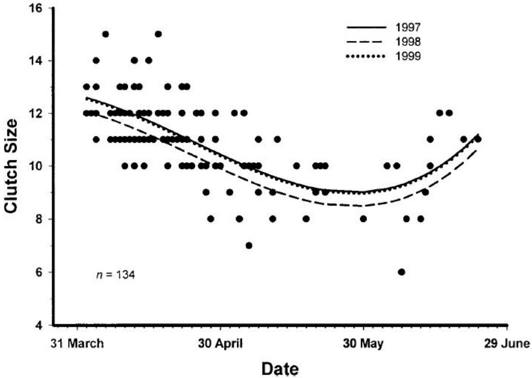
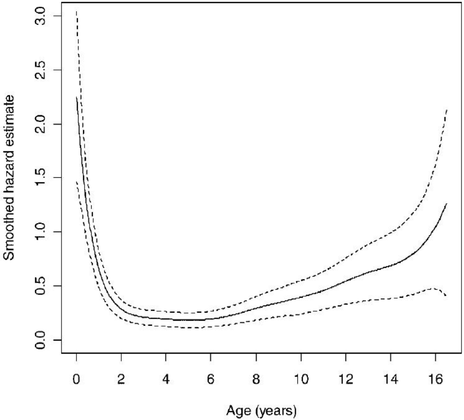
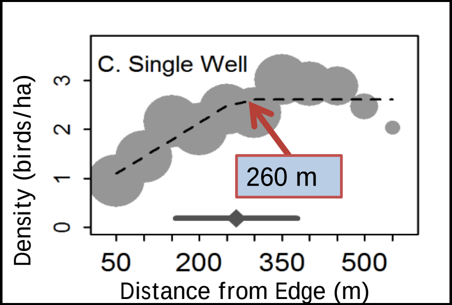


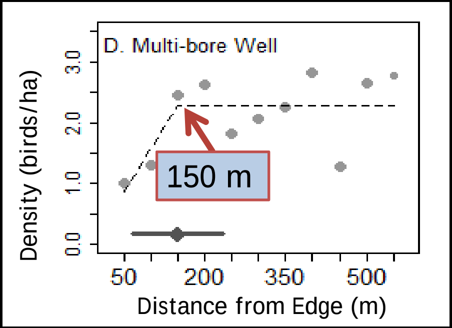
FIG. 2. Mallard clutch size in nest structures was modeled as having a curvilinear relationship to nest initiation date in western Minnesota, 1997–1999.

Age-specific Hazard for White-tailed Deer



Grassland Birds Combined





Linear Models

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

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

or

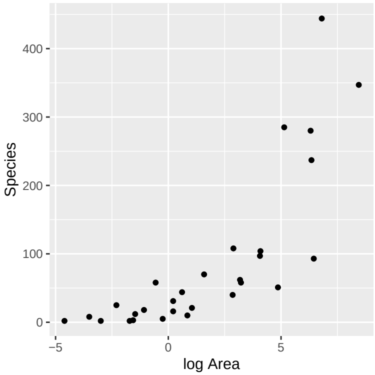
$$Y_i = \beta_0 + X_{i,1}\beta_1 + X_{i,2}\beta_2 + \ldots + \epsilon_i$$

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_grey(base_size=20)
```



[1] http://www.ibiblio.org/pub/academic/biology/ecology+evolution/teaching/v

Modeling Non-Linear Relationships

- Polynomials (e.g., poly(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*:

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

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

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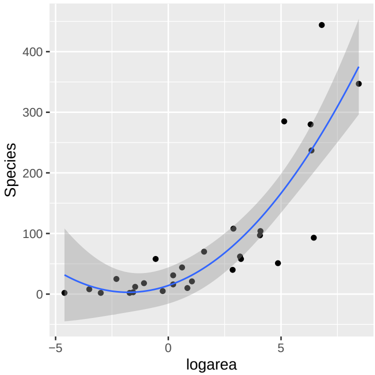
$$\sqrt{Y_i} = \beta_0 + log(X_i)\beta_1 + \ldots + \epsilon_i$$

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!]

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

```r
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

```r
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:
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```
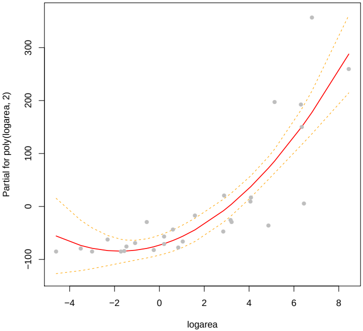

Polynomials: component + residual plot

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



Hypothesis Testing

```r
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
```

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---
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
```

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.

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

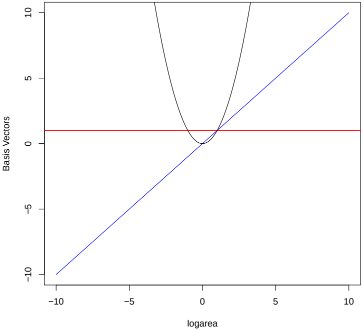
$$b_j(X_i) = 1, X, X^2, X^3, \ldots$$

```r
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

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

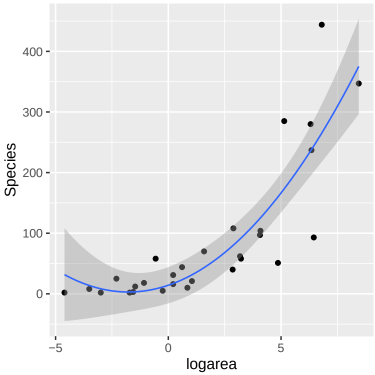


$E[Y|X]$ is given by a linear combination of a horizontal line (1), a line through the origin (X), a quadratic centered on the origin (X^2), etc.

Species-Area relationship

$$Species_i = 14.15 + 12.62X_i + 3.56X_i^2$$

```
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:

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

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

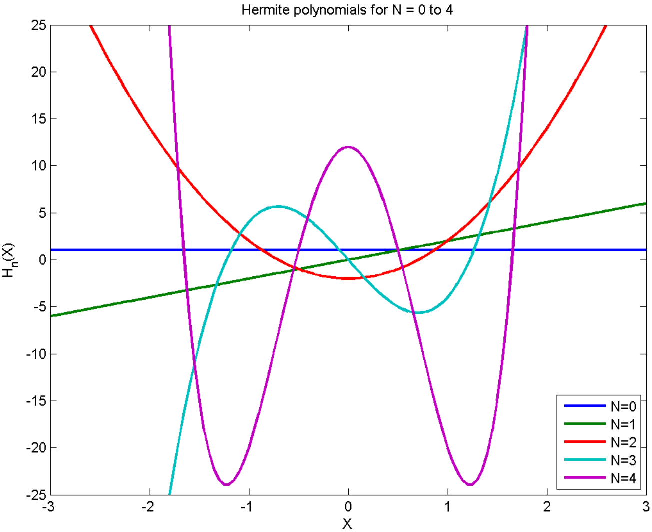
Polynomials

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

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

Polynomials



Orthogonal Polynomials

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

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

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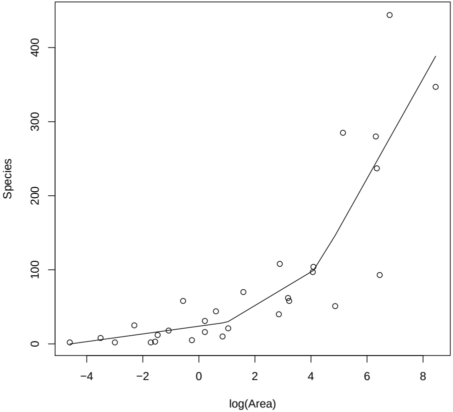
Centering and scaling X can help.

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

Splines

Species-Area relationship

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



Splines

Splines are piecewise polynomials used in curve fitting.

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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)
```

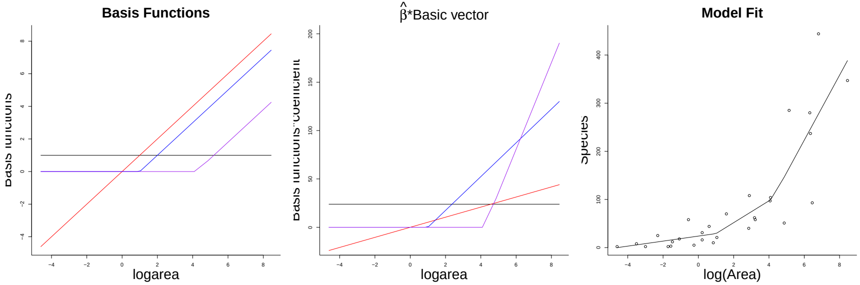
```
Call:
lm(formula = Species ~ logarea + logarea.1 + logarea.4.2, data = gala)

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



- Left = Basis Functions
- Middle = Basis Functions * regression coefficient
- Right = Fitted Model

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 Dth 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)

Cubic Regression Splines

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  - 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.

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

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

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

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

Splines

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

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

Basis functions: Splines

Truncated power basis:

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

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- Can be poorly behaved in the tails

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- 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 refered to as *boundary knots*)
- Requires fewer model df (number of knots -1 = number of interior knots + 1)

Span: Splines

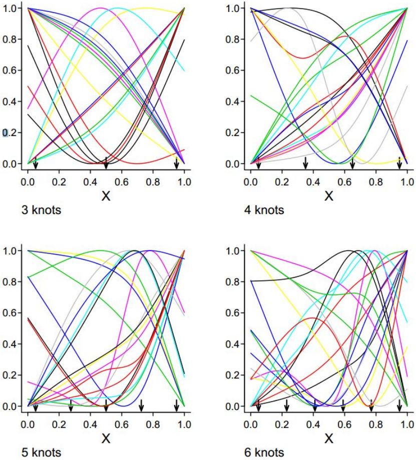


Figure 2.3: Some typical restricted cubic spline functions for $k = 3, 4, 5, 6$. The y–axis is $X\beta$. Arrows indicate knots. These curves were derived by randomly choosing values of β subject to standard deviations of fitted functions being normalized.

Natural Splines

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

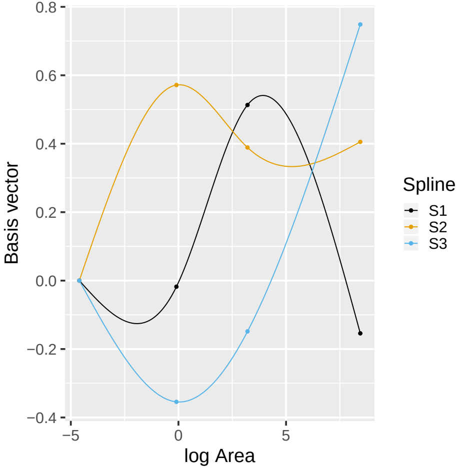
```
Call:
lm(formula = Species ~ ns(logarea, df = 3), data = gala)

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




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

```
[1] -0.09393711  3.20877345
```

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

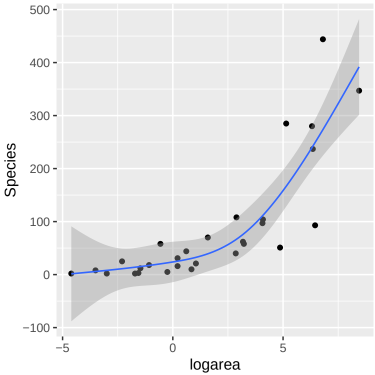
```
[1] -4.605170  8.448769
```

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

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

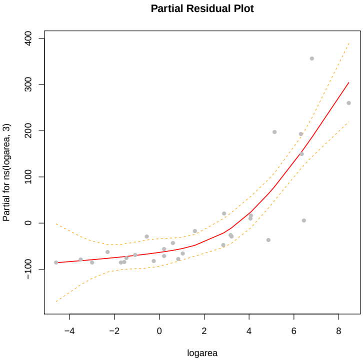
Natural Splines

```
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

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



Compare fit to that of linear model

```
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.

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- 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 $n > 100$

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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

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

```
[1] -0.09393711  3.20877345
```

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

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

```r
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

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

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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

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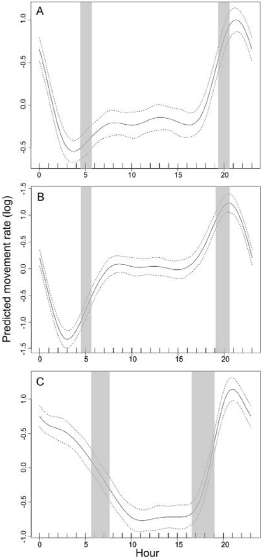
- Other basis functions can be used to fit 'smooth surfaces' (allowing for interactions between variables)
  - tensor splines, thin plate splines, etc…
- Can include interactions (separate smooth for each level of a categorical variable)

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

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