An Introduction to R for the Geosciences: Regression

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Simple linear regression

- Simple linear regression is a statistical model that assumes a linear relationship between a continuous response variable y and one or more, usually continuous, predictor variables, $X = x_1, \ldots, x_n$
- Three major purposes of such models
  - to describe the linear relationship between y and X
  - to determine how much variation (uncertainty) in y can be explained by the relationship with X, and
  - to predict new values of y from new values of X
- A linear model is linear in its parameters only — the fitted response can be non-linear in the English sense of the word

Simple linear regression

- Consider first the case of a single predictor variable x and its relationship to y
- A suitable form for such a model is

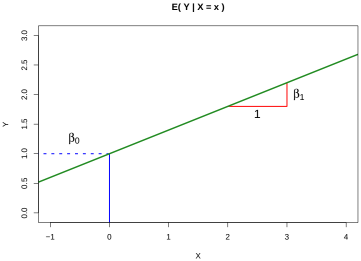
$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

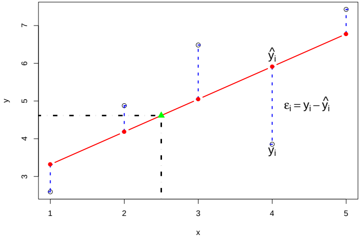
- We need to estimate two parameters (β_0 and β_1)
- β_0 is the intercept, the mean of the probability distribution of y when x is 0
- β_1 is often called the slope, it measures the rate of change in y for a per unit change in x
- Estimate the parameters using least-squares, solving this model by minimising Residual Sum of Squares

$$RSS = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

Least-squares

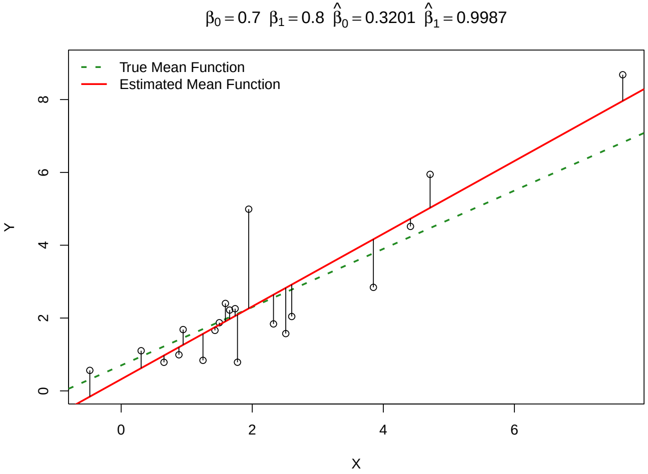
- $\hat{\beta}_0$ is the estimate of the intercept
- $\hat{\beta}_1$ is the estimate of the slope
- Observed points (y_i) are open circles
- Fitted points $(\hat{y}_i)$ are filled circles
- Fitted model/line is solid line through $\hat{y}_i$
- Dashed lines between y_i and $\hat{y}_i$ are the residuals (ε_i)
- Thick black line shows prediction of $\hat{y}_{new}$ given a new x value of 2.5





Least-squares

- Data generated from true mean function
- Least squares estimates of mean function



Least-squares

- Data are 20 observations generated from the following model

$$y_i = 0.7 + 0.8x_i + \varepsilon_i$$

$$\varepsilon_i \sim N(\mu = 0, \sigma = 1)$$

- Fitted model gives $\hat{\beta}_0 = 0.3201$ and $\hat{\beta}_1 = 0.9987$
- F-ratio for this fitted model is 66.43, which has a p-value of > 0.0001 from a F distribution with 1 and $n - 2$ (20) degrees of freedom
- This is equivalent of testing our model against the Null model (null hypothesis) that

$$y_i = \beta_0 + \varepsilon_i$$

- where β_0 is just the sample mean, $\bar{y_i}$, i.e. that there is no variation in y given x

Assumptions of least squares regression

1. The linear model correctly describes the functional relationship between y and X
   - If violated the estimate of predictor variances (σ^2) will be inflated
   - Incorrect model specification can show itself as patterns in the residuals
2. x_i are measured without error
   - Allows us to isolate the error component as random variation in y
   - Estimates $\hat{\beta}$ will be biased if there is error in X — often ignored!
3. For any given value of x_i, the sampled y_i values are independent with normally distributed errors
   - Independence and normality of errors allows us to use parametric theory for confidence intervals and hypothesis tests on the F-ratio.
4. Variances are constant along the regression line/model
   - Allows a single constant variance σ^2 for the variance of the regression line/model
   - Non-constant variances can be recognised through plots of residuals (amongst others) — i.e. residuals get wider as the values of y increase.

Fitting linear models in R

Typical model call & output from R. Next few slides explain the salient results

```
> mod <- lm(Age ~ Depth, data = agedat)
> summary(mod)

Call:
lm(formula = Age ~ Depth, data = agedat)

Residuals:
     Min       1Q   Median       3Q      Max
-15.3808  -7.7115   0.7053   6.1577  16.7818

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  21.2480     3.5626   5.964 2.02e-06 ***
Depth         5.5760     0.3208  17.384  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 9.131 on 28 degrees of freedom
Multiple R-squared: 0.9152, Adjusted R-squared: 0.9122
F-statistic: 302.2 on 1 and 28 DF,  p-value: < 2.2e-16
```

Fitting linear models in R

- `Estimate` is β_j, the model coefficients, on log scale (base e)
- For 1m increase in sediment `Depth`, sediment `Age` decreases by 5.576kyrs
- `t-value` is the t statistic, the ratio of the estimate and its standard error $t = \frac{\hat{\beta}_j}{\hat{\mathrm{se}}_j}$
- p-value is probability of achieving a t as large or larger than the one observed under null hypothesis
- Intercept of interest — sediment age at 0m sediment depth

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  21.2480     3.5626   5.964 2.02e-06 ***
Depth         5.5760     0.3208  17.384  < 2e-16 ***
```

Fitting linear models in R

- Residual standard deviation $\hat{\sigma} = 9.131$; a measure of the variance of the residuals
- r^2 is the coefficient of determination, the ratio of the variance explained to the total variance; a measure of how much variance is explained

$$r^2 = \frac{\mathrm{SS}_{\mathrm{regression}}}{\mathrm{SS}_{\mathrm{regression}} + \mathrm{RSS}} = 1 - \frac{\mathrm{SS}_{\mathrm{residual}}}{\mathrm{SS}_{\mathrm{total}}}$$

- Adjusted r^2 takes into account number of predictors in the model

$$r^2_{\mathrm{adj}} = 1 - \frac{\mathrm{SS}_{\mathrm{residual}}/[n-(p+1)]}{\mathrm{SS}_{\mathrm{total}}/(n-1)}$$

- If we added a redundant predictor to model r^2 would increase. r^2_{adj} attempts to control for this phenomenon

```
Residual standard error: 9.131 on 28 degrees of freedom
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F-statistic: 302.2 on 1 and 28 DF,  p-value: < 2.2e-16
```

Fitting linear models in R

- F is the F-ratio, the ratio of the regression and residual variances (Mean squares)

$$F = \frac{\sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 / p}{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 / [n - (p+1)]} = \frac{\mathrm{MS}_{\mathrm{regression}}}{\mathrm{MS}_{\mathrm{residual}}}$$

- Probability of F greater than or equal to observed from F-distribution with p and $n - (p+1)$ degrees of freedom

```
> anova(mod)
Analysis of Variance Table

Response: Age
          Df  Sum Sq Mean Sq F value    Pr(>F)
Depth      1 25195.9 25195.9   302.2 < 2.2e-16 ***
Residuals 28  2334.5    83.4
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Fitting linear models in R — Hypothesis testing

- t tests are tests the H_0 that $\hat{\beta}_j = 0$
- F tests the ratio of variance explained to unexplained
- With single predictor, t test for `length` and F of model are equivalent
- More generally we can think of F as comparing

$$y_i = \beta_0 + \varepsilon_i$$

with

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

```
> mod0 <- lm(Age ~ 1, data = agedat)
> anova(mod0, mod) ## same as anova(mod)
Analysis of Variance Table

Model 1: Age ~ 1
Model 2: Age ~ Depth
  Res.Df     RSS Df Sum of Sq     F    Pr(>F)
1     29 27530.4
2     28  2334.5  1     25196 302.2 < 2.2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

R's model formula

- R uses a slightly modified version of the Wilkinson-Rogers (Wilkinson & Rogers (1973; Applied Statistics **22**;392–399) notation to symbolically describe statistical models

```
mod <- lm(Y ~ x1 + x2, data = mydata)
```

- Intercept implied; suppress with `- 1` or `+ 0`

```
mod <- lm(Y ~ x1 + x2 - 1, data = mydata)
```

- Interaction terms with `a : b`

```
mod <- lm(Y ~ x1 + x2 + x1:x2, data = mydata)
```

- Can be simplified using `a * b`

```
mod <- lm(Y ~ x1 * x2, data = mydata)
```

- Shortcut to add all variables to model is `.` (Careful!)

```
mod <- lm(Y ~ ., data = mydata)
```

- Polynomials via `I(x^2)` or `poly(x, 2)`

```
mod <- lm(Y ~ x + I(x^2), data = mydata)
mod <- lm(Y ~ poly(x, 2), data = mydata)
```

R's model formula

- Note the use of the `data` argument. This is a data frame (or list) containing the variables to include in the model

  ```
  mod <- lm(Y ~ x1 + x2, data = mydata)
  ```

- You never want to do this

  ```
  mod <- lm(mydata$Y ~ mydata$x1 + mydata$x2)
  ```

- Apart from taking longer to type, the `predict()` method won't work easily
- Can include functions in formula as `poly(x, 2)` earlier

  ```
  mod <- lm(Y ~ log(x), data = mydata)
  ```

- Better to do this if you can than transform data & store both transformed and untransformed variable in your data frame. Not least because `predict()` just works
- You can exclude variables too

  ```
  mod <- lm(Y ~ x1 + x2 - x3, data = mydata)
  ```

Multiple regression

- The simple regression model readily generalises to the situation where we have m predictors not just one.

$$y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_m x_m + \varepsilon$$

- Now we have $m + 1$ parameters to estimate, one for intercept and one each for the m predictors x_m
- It is tedious to write all that out, so we collect the β_m into a vector β and all the predictors (including the intercept, a vector of 1s) into the model matrix, X, then rewrite the model as

$$y = \mathbf{X}\beta + \varepsilon$$

Akaike information criterion

- Akaike information criterion (AIC) is an index of fit that takes account of the parsimony of the model by penalising for the number of parameters
- The more parameters in the model the better the fit — if you have as many parameters as data points then the fit is perfect but the model has no explanatory power! A Trade-off.
- AIC is useful as it explicitly penalises any superfluous parameters in the model by adding $2p$ where p is the number of parameters to the variance or deviance of the model.

$$\mathrm{AIC} = -2 \times \max \mathrm{loglikelihood} + 2p$$

- Associated is Bayes information criterion (BIC), which applies a stronger penalty of $p \log n$, where n is number of observations
- For linear regression the $-2 \times \max \mathrm{loglikelihood}$ is $n \log(RSS/n) + \mathrm{constant}$, where RSS is the residual sums of squares.

Akaike information criterion

- We use AIC and BIC to compare two or more nested models
- Nested means that one model is a subset of the other
- The model with the smallest AIC or BIC is to be preferred
- Note that you can get negative values for AIC and BIC. This is fine, just go for the smallest value: e.g. -21.5 is better than -15.4
- Difference in AIC of 2 is expected with a redundant parameter
- Models with AIC differing by 2 or less are effectively the same
- `AIC()` & `BIC()` methods can be used to extract IC from fitted model objects

```
> AIC(mod)
[1] 221.7669
> BIC(mod)
[1] 225.9705
```

ANOVA — the Analysis of Variance

- ANOVA is a general statistical technique for partitioning and analysing the variation in a continuous response variable
- Earlier we used ANOVA to partition the variance in a response variable into components explained by explanatory variables and a residual component not explained by the regression model
- A slightly more restricted view of ANOVA is that it is a technique for partitioning the variation in a response variable into that explained or unexplained by one or more categorical predictor variables or factors
- The categories of each factor are the groups or experimental treatments
- Often the focus is on comparing the mean of the response variable between groups
- We won't dwell too much on the distinction between regression and ANOVA — they are effectively the same and in R we use the same fitting function, e.g. `lm()`

Simple one-way ANOVA

- One-way ANOVA designs deal with only a single factor or predictor variable
- The single factor comprises 2 or more groups
- Medley & Clements (1998) studied the response of diatom communities to heavy metals (esp. Zinc, Zn) in streams in the Rocky Mountain region of Colorado, USA
- They sampled a number of stations (4–7) on six streams known to be polluted by heavy metals
- Several variables were measured at each station, inc. Zn concentration, diatom species richness and diversity, and proportion of diatom cells belonging to the diatom *Achnanthes minutissima*
- Zn concentration used to group sites into four categories;
- Is there a difference in species diversity between the four Zn categories?

Rocky mountain diatoms

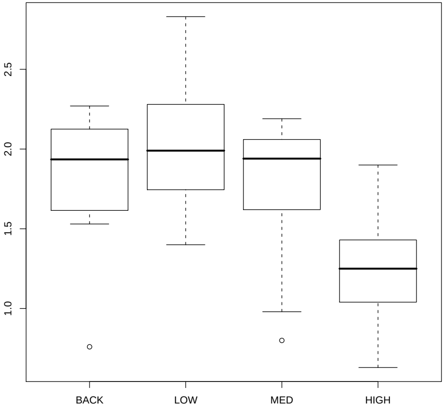
```
> diatom <- read.csv("medley.csv")
> diatom$ZINC <- factor(diatom$ZINC, levels = c("BACK","LOW","MED","HIGH"))
> ## Drop some superfluous columns
> diatom <- diatom[, 1:3]
> head(diatom)
  STREAM ZINC DIVERSITY
1  Eagle BACK      2.27
2  Eagle HIGH      1.25
3  Eagle HIGH      1.15
4  Eagle  MED      1.62
5   Blue BACK      1.70
6   Blue HIGH      0.63
> str(diatom)
'data.frame':   34 obs. of  3 variables:
 $ STREAM   : Factor w/ 6 levels "Arkan","Blue",..: 4 4 4 4 2 2 2 2 2 2 ...
 $ ZINC     : Factor w/ 4 levels "BACK","LOW","MED",..: 1 4 4 3 1 4 1 1 4 3 ...
 $ DIVERSITY: num  2.27 1.25 1.15 1.62 1.7 0.63 2.05 1.98 1.04 2.19 ...
> table(diatom$ZINC)

BACK  LOW  MED HIGH 
   8    8    9    9 
> table(diatom$STREAM)

Arkan  Blue Chalk Eagle Snake Splat 
    7     7     5     4     5     6 
> with(diatom, table(ZINC, STREAM))
      STREAM
ZINC   Arkan Blue Chalk Eagle Snake Splat
  BACK     0    3     0     1     1     3
  LOW      5    0     2     0     0     1
  MED      2    2     1     1     1     2
  HIGH     0    2     2     2     3     0
```

Rocky Mountain diatoms

```
> boxplot(DIVERSITY ~ ZINC, data = diatom)
```



Rocky Mountain diatoms — ANOVA

```
> zn.lm1 <- lm(DIVERSITY ~ ZINC, data = diatom)
> summary(zn.lm1)

Call:
lm(formula = DIVERSITY ~ ZINC, data = diatom)

Residuals:
     Min       1Q   Median       3Q      Max 
-1.03750 -0.22896  0.07986  0.33222  0.79750 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  1.79750    0.16478  10.909 5.81e-12 ***
ZINCLOW      0.23500    0.23303   1.008   0.3213    
ZINCMED     -0.07972    0.22647  -0.352   0.7273    
ZINCHIGH    -0.51972    0.22647  -2.295   0.0289 *  
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1 

Residual standard error: 0.4661 on 30 degrees of freedom
Multiple R-squared: 0.2826, Adjusted R-squared: 0.2108 
F-statistic: 3.939 on 3 and 30 DF,  p-value: 0.01756 

> anova(zn.lm1)
Analysis of Variance Table

Response: DIVERSITY
          Df Sum Sq Mean Sq F value  Pr(>F)  
ZINC       3 2.5666  0.8555  3.9387 0.01756 *
Residuals 30 6.5164  0.2172                  
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1 
```

Rocky Mountain diatoms — different parametrisation

- Previous model (`zn.lm1`) contained an intercept
- To maintain identifiability, need to set one level of `ZINC` as reference level and express model as differences in mean diversity from this reference level
- If we re-parametrise and drop the intercept, the estimates are the group means

```
> zn.lm0 <- lm(DIVERSITY ~ ZINC - 1, data = diatom)
> coef(zn.lm0)
ZINCBACK  ZINCLOW  ZINCMED ZINCHIGH
1.797500 2.032500 1.717778 1.277778
> with(diatom, aggregate(DIVERSITY, list(ZINC = ZINC), mean))
  ZINC        x
1 BACK 1.797500
2  LOW 2.032500
3  MED 1.717778
4 HIGH 1.277778
```

Rocky Mountain diatoms — dummy variable coding in R

- Both models use Treatment contrasts
- Normally, one level is set as baseline and dropped, and contrasts code so as to reflect differences in that level from reference level
- Other contrasts are available, such as Helmert contrasts, see `?contrasts`

```
> model.matrix(zn.lm1)
   (Intercept) ZINCLOW ZINCMED ZINCHIGH
1            1       0       0        0
2            1       0       0        1
3            1       0       0        1
4            1       0       1        0
5            1       0       0        0
6            1       0       0        1
7            1       0       0        0
8            1       0       0        0
9            1       0       0        1
10           1       0       1        0
....
attr(,"assign")
[1] 0 1 1 1
attr(,"contrasts")
attr(,"contrasts")$ZINC
[1] "contr.treatment"
```

Outliers

- Outlier — observation which is inconsistent with the rest of the observations in a sample.
- An observation can be an outlier due to the response variable(s) or one or more of the predictor variables having values outside their expected limits.
- Identify outliers at EDA stage for investigation and evaluation, *not* rejection and deletion.
- An outlier may result from
  - incorrect measurement,
  - incorrect data entry,
  - transcription error,
  - recording error,
- Outliers are model dependent
- Two main concepts
  - Leverage — Potential for an outlier to be influential
  - Influence — Observation is influential if its deletion substantially changes the results

Leverage measures

Projection or Hat matrix

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}$$

where $\mathbf{X}$ is the $n \times p$ matrix of x values, the parameters in the model. $\mathbf{H}$ is an $n \times n$ matrix.

Hat matrix

$$\mathbf{H} = \begin{vmatrix} h_{11} & h_{12} & \dots & h_{1n} \\ h_{21} & h_{22} & \dots & h_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ h_{n1} & h_{n2} & \dots & h_{ii} \end{vmatrix}$$

- Hat matrix is so called because it puts a hat on $\mathbf{Y}$: $\hat{\mathbf{Y}} = \mathbf{HY}$.
- Leverage of an observation i is denoted h_{ii} — the ith element of the diagonal of $\mathbf{H}$.
- Leverage ranges from $1/n$ to 1.
- Observation has high leverage if h_{ii} is 2 or 3 times $h = (k+1)/n$, where $k+1$ is number of coefficients (inc. the constant term).
- As $h_{ii} \rightarrow 1$, x_i may dominate model.

Influence measures — DFBETAS

- An observation that combines "outlyingness" with high leverage exerts an influence on the estimated regression coefficients
- If such an observation is deleted from the analysis, the estimated coefficients change substantially.

dfbeta

$$\mathrm{dfbeta}_{ij} = \beta_{j(-i)} - \beta_j$$

dfbetas

$$\mathrm{dfbetas}_{ij} = \frac{\beta_{j(-i)} - \beta_j}{s_{r(i)}\sqrt{(\mathbf{X}^\mathbf{T}\mathbf{X})_{jj}}}$$

β_j slope of regression; $\beta_{j(-i)}$ slope when x_i deleted; $s_{r(i)}$ residual SD when x_i deleted; $(\mathbf{X}^\mathbf{T}\mathbf{X})_{jj}$ the RSS

- dfbeta_{ij} assesses the impact on the jth coefficient of deleting the ith observation.
- The dfbeta_{ij} are expressed in the metric of the coefficient.
- A standardised version, $\mathrm{dfbetas}_{ij}$ divides dfbeta_{ij} by the standard error of β_j.
- Influential observations have $\mathrm{dfbetas}_{ij} \geq 2/\sqrt{n}$

Influence measures — Cook's distance

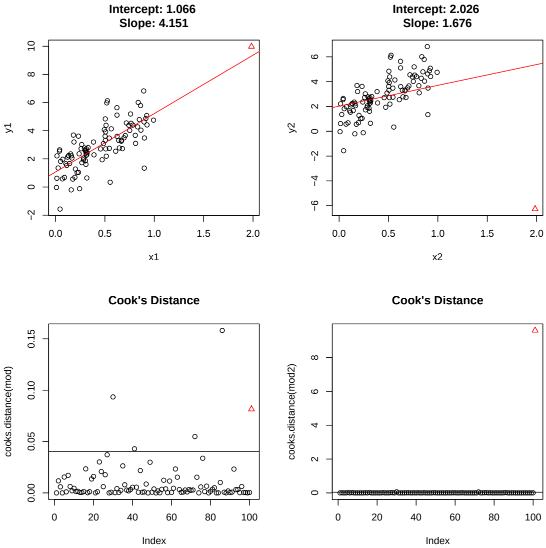
Cook's Distance

$$D_i = \frac{e_i^2}{s^2(k+1)} \times \frac{h_i}{1-h_i}$$

where e^2 is the squared residual for x_i; s^2 is the variance of the residuals; h_i is the hat value for x_i

- One problem with $\mathrm{dfbetas}_{ij}$ is that there are so many numbers!
- One for each observation for every β_j (inc. the constant); $n \times (k+1)$.
- D_i is a scale invariant measure of distance between β_j and $\beta_{j(-i)}$.
- The first fraction is a measure of "outlyingness", the second of leverage.
- $D_i \geq 4/(n-k-1)$ suggested as a cut-off for high values of D_i.

Leverage and influence; example



Influence measures in R

- Several functions extract influence measures from fitted models; see `?influence.measures` for details

```
> head(cooks.distance(mod))
           1            2            3            4            5            6 
0.0002843771 0.1987126125 0.2084128586 0.1427614594 0.0092847760 0.0084433941 
> head(hatvalues(mod))
         1          2          3          4          5          6 
0.14468969 0.11994389 0.09996128 0.09991500 0.08264498 0.05635662 
> influence.measures(mod)
Influence measures of
	 lm(formula = Age ~ Depth, data = agedat) :

      dfb.1_ dfb.Dpth   dffit cov.r   cook.d    hat inf
1  -0.023418  0.02055 -0.0234 1.257 2.84e-04 0.1447   *
2  -0.652525  0.55579 -0.6541 0.981 1.99e-01 0.1199    
3   0.675657 -0.55622  0.6813 0.896 2.08e-01 0.1000    
4  -0.546052  0.44948 -0.5506 0.985 1.43e-01 0.0999    
....
```

Model selection

- Where we have several candidate covariates for inclusion in a model, we face the problem of selecting a minimal, adequate model
- A minimal, adequate model is one that is complex enough to provide sufficient fit to the observed response but no more complex than is necessary
- Several automated techniques available to help
    1. Best subsets regression — fit all combination of covariates and choose the best model
    2. Forward selection — start with no covariates, add the covariate that improves fit most, repeat till no covariate results in significant improvement
    3. Backwards elimination — as above but start with all covariates and remove the worst variable as long as the model is not made significantly worse
    4. Stepwise regression (forward selection and backward elimination)
- Regardless of method used to select a minimal model, you must be aware that these techniques are not a panacea
- p-values from tests on the selected model do not account for the selection procedure; anti-conservative, too many variables selected

Stepwise regression in R

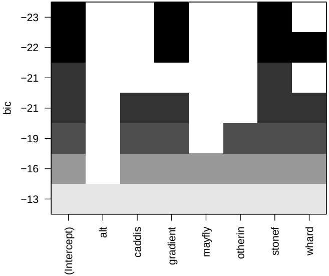
- Base R contains several functions for stepwise selection
  - `step()`
  - `add1()`
  - `drop1()`
- The latter two allow manual selection by single-term addition (`add1()`) or deletions (`drop1()`)
- `step()` is fully automated
- All do selection using AIC not p values
- Package **MASS** contains
  - `stepAIC()`
  - `addterm()`
  - `droptrem()`
- Uses AIC for selection also
- Practical will contain examples of all of these

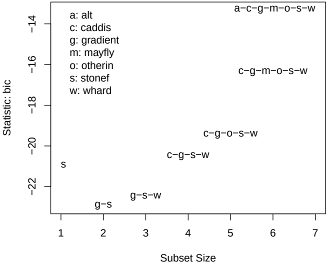
Best subset regression

- Identifies the best model of each size
- Can use many statistics but AIC and BIC are commonly used

$$\text{AIC} = -2 \times \log(\mathcal{L}(\beta_i)|\text{data}) + kp$$

- k is a penalty on complexity; AIC: $k = 2$; BIC: $k = \log(n)$
- p is number of parameters in model.
- Best subsets is available in package **leaps**





Subset selection and Shrinkage

- Subset selection often used for 2 reasons:
  - Interpretation — Smaller subset of predictors with strongest effects on response y may be easier to interpret and explain
  - Prediction accuracy — LSQ estimates have low bias but large variance. Can sometimes improve prediction accuracy by shrinking the coefficients or setting some to zero. In doing so we sacrifice a bit of bias
- Subset selection leads to a small set of interpretable predictors, with possibly lower error (MSE) than the full model
- Subset selection is a discrete process — predictors are either **in** the model, or **out**
- As a result, this subset model often exhibits high variance, which limits the possible improvement in error
- Shrinkage methods are more continuous than subset selection and do not suffer from high variability to the same degree

Stepwise selection & best-subsets

- Stepwise selection is a combination of forward selection and backward elimination steps
- Forward selection: start with no terms in model & sequentially add the variable that best improves the model
- Backward elimination: start with the full model & sequentially remove the variable that effects the model least
- Best-subsets: consider all possible combinations of models (variables) and select the best model for a range of model sizes or select the best model overall
- Several problems with this however:
  - selection bias in the estimates of the model coefficients $\hat{\beta}_i$
  - increased variance of the selected model, and
  - bias in the standard errors of $\hat{\beta}_i$

Selection bias

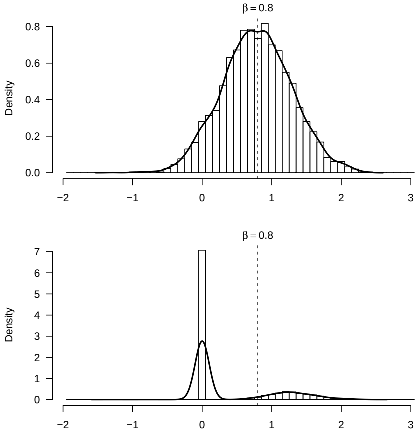
- Selection bias occurs in the estimates of the model coefficients $\hat{\beta}_i$ in the selection methods
- This bias arises from the effective imposition of a hard threshold on the size of the $\hat{\beta}_i$
- $\hat{\beta}_i = 0$ when ith variable is not selected
- Extreme example from Whittingham et al (2006); 5000 data sets $(n = 10)$ drawn from the model:

$$y_i = 1 + 0.8x_i + \varepsilon_i$$

- $\beta = 0.8$, $x_i = 1, 2, \ldots, 10$, $\varepsilon_i \sim N(\mu = 0, \sigma_i = 1)$
- Selection threshold applied of $\hat{\beta} = 0$ where $p > 0.05$

(top) Distribution of $\hat{\beta}$ when OLS applied to each data set.

(bottom) Distribution of $\hat{\beta}$ when significance threshold applied



Ridge regression

- Ridge regression shrinks the coefficients via imposition of a penalty to restrict their size
- Ridge regression coefficients minimises a penalised RSS

$$\beta_{\mathrm{ridge}} = \underset{\beta}{\mathrm{argmax}} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}$$

or

$$\beta_{\mathrm{ridge}} = \underset{\beta}{\mathrm{argmax}} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2$$

subject to

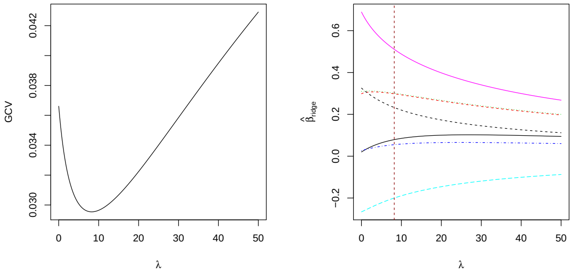
$$\sum_{j=1}^{p} \beta_j^2 \leq t$$

Ridge regression

- With collinear variables, $\hat{\beta}_{\mathrm{LSQ}}$ are poorly determined and have high variance
- One variable can have a large positive coefficient, counteracted by variable with which it is correlated having a large negative coefficient
- Imposing a constraint on size of the coefficients can alleviate this
- Predictors are standardised before running ridge regression
- Intercept β_0 is not subject to the penalty
- Ridge regression shrinks components in the predictors that have low variance (explain low amounts of the variance in $\mathbf{X}$)

Ridge regression

- Need to select a value for the penalty λ, or for the limit on the size of the coefficients t
- Choose these on basis of GCV criterion or CV
- $\lambda = 0$ gives no shrinkage and $\hat{\beta}_{\mathrm{ridge}} = \hat{\beta}_{\mathrm{LSQ}}$
- Ridge regression applied to the Dipper breeding density data:



The Lasso

- The Lasso is a shrinkage method like the ridge regression but with important differences — namely the Lasso can perform variable selection as well as shrink coefficients
- The lasso finds coefficients $\hat{\beta}_{lasso}$ that minimise a penalised RSS

$$\hat{\beta}_{\text{lasso}} = \underset{\beta}{\text{argmax}} \left\{ \frac{1}{2} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}$$

or

$$\beta_{\text{lasso}} = \underset{\beta}{\text{argmax}} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2$$

subject to

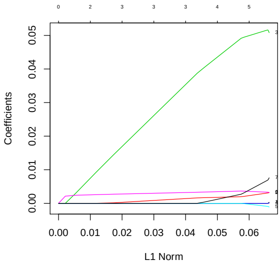
$$\sum_{j=1}^{p} |\beta_j| \leq t$$

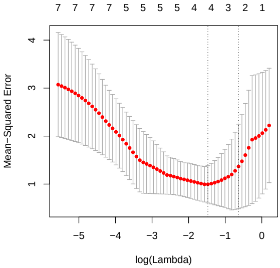
The Lasso

- The predictors are standardised prior to analysis and the intercept is not subjected to the penalty term
- Because of the different penalty, if t is sufficiently small (or λ sufficiently large) some of the $\hat{\beta}_{lasso}$ can be shrunk to 0
- This has the effect of selecting those variables with zero coeffcients out of the model
- Optimal values for t or λ are chosen using GCV or CV to find those that minimise the prediction error
- Unlike ridge regression, the lasso doesn't penalise sets of low variance or correlated variables to the same extent, however...
- It does do feature selection for us

The Lasso

- Lasso applied to Dipper density data
- Minimum CV error at $\lambda = 0.276$, simpler model within 1 standard error at $\lambda = 0.581$
- 4 predictors have positive coefficients at best model, 3 at the model with 1 standard error
- Gradient (0.019), Stonefly (0.0028), Caddis (0.0004)





The Elastic Net

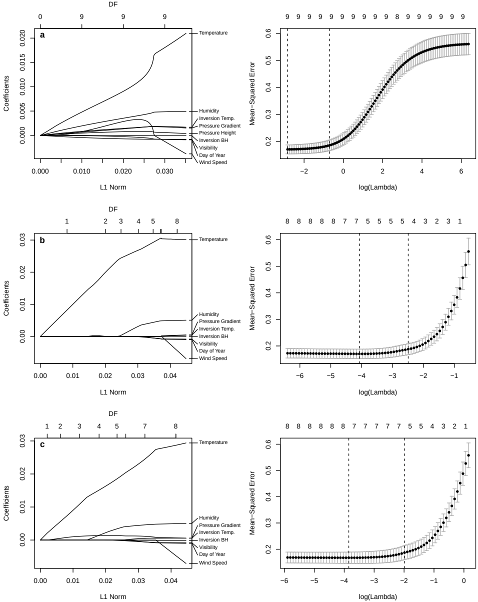
- Ridge regression shrinks all coefficients, proportionally, whilst the Lasso transforms each coefficient by constant factor λ and truncates at zero
- Ridge regression shrinks together the coefficients of correlated data, whilst the Lasso can select or remove coefficients from the model
- Useful if these two properties could be combined
- This is what the Elastic Net penalty does
- Find coefficients $\hat{\beta}_{\text{elastic}}$ that minimise the penalised RSS with penalty

$$\lambda \sum_{j=1}^{k} (\alpha \beta_j^2 + (1 - \alpha)|\beta_j|)$$

- α controls the relative weighting of the ridge-like and lasso-like properties
- Find optimal values of λ and α via a grid search over the parameters using CV and 1se rule

Comparison of shrinkage methods: Ozone data

- Various shrinkage methods applied to predict Ozone concentration using climatic variables
- Left panels show full regularisation paths of $\hat{\beta}_i$ for (a) ridge, (b) lasso, and (c) elastic net
- Right panels show k-fold CV errors for increasing (left to right) penalty
- Dashed vertical lines indicate best model (lowest CV error) and the smallest model within 1 standard error of the best model (right-most dashed line)
- Notice how ridge regression does not perform selection but shrinks correlated variables (Temperature & Wind Speed)
- Lasso performs selection; note difference in paths for Temperature & Wind Speed
- Elastic net ($\alpha = 0.5$) combines both; most similar here to Lasso



Degrees of freedom for shrinkage models

- The degrees of freedom used in finding the fitted values $\mathrm{df}(\hat{y})$ is an important of model complexity
- If we *a priori* present a set of k predictors to linear regression, then that model uses $k+1$ (for the intercept) $\mathrm{df}(\hat{y})$
- If we do best subset regression, software assumes we have used k df but really we used many more than k
- What about techniques like the lasso and ridge regression?
- Effective degrees of freedom given by

$$\mathrm{df}(\hat{y}) = \frac{1}{\sigma^2} \sum_{i=1}^{n} \mathrm{Cov}(\hat{y}_i, y_i)$$

- The harder we try to fit the response y_i, the larger their covariance with the fitted values and therefore the more degrees of freedom we have used

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- The harder we try to fit the response y_i, the larger their covariance with the fitted values and therefore the more degrees of freedom we have used
- This equation works for ordinary regression (it will give k degrees of freedom)
- It works for ridge regression and for the lasso
- In theory this should also work for best subsets regression, but we don't have a closed form equation for estimating $\mathrm{df}(\hat{y})$ in that case
- Highlights the problem of determining the real $\mathrm{df}(\hat{y})$ used if we do best subsets or forward selection / backwards elimination

Multicollinearity redux - VIF

- Variance inflation factor (VIF; V) is related to the sampling variance of a regression coefficient

$$\hat{V}(\hat{\beta}_j) = \frac{s^2}{(n-1)s_j^2} \times \frac{1}{1-R_j^2}$$

  where s^2 is estimate error variance, s_j^2 is sample variance of jth covariate

- $\mathrm{VIF} = \frac{1}{1-R_j^2}$ is the variance-inflation factor and is a function of the multiple correlation R_j from regression of jth covariate on the other covariates
- $\sqrt{\mathrm{VIF}}$ is a measure of by how much the confidence interval for $\hat{\beta}_j$ is expanded relative to the case where uncorrelated data are used
- $\mathrm{VIF} >\sim 10$ then a covariate is largely explain by other covariates in the model

Multicollinearity redux

- Ridge regression and the lasso estimate biased coefficients
- We accept this extra bias because we attempt to offset the increased variance that complex models and correlated covariates causes
- None of the approaches we talked about is universally a panacea or solution to collinearity
- The real solution is to collect new data so that variables aren't collinear
- Biased estimation methods *may* cause problems worse that collinearity!
- Really, does collinearity actually matter? If we estimate $\hat{\beta}_j$ with sufficient precision then collinearity doesn't matter
- If we can't achieve sufficient precision because of collinearity, this knowledge is only useful if we can redesign the study and collect uncorrelated data
- Think (!) about which terms you introduce to a model

Selected texts

- Fox, J (2008) *Applied regression analysis and generalized linear models*. Sage. (Chapter 13)
- Hastie, T., Tibshirani, R., & Friedman, J. (2010) *The elements of statistical learning*. 2nd Edition. Springer. (Chapter 3). Available from: www.stanford.edu/~hastie/pub.htm
- Whittingham, M.J. et al (2006) Why do we still use stepwise modelling in ecology and behaviour? *Journal of Animal Ecology* **75**:1182–1189
- Murtaugh, P.A. (2009) Performance of several variable-selection methods applied to real ecological data. *Ecology Letters* **12**:1061–1068
- Dahlgren, J.P. (2010) Alternative regression methods are not considered in Murtaugh (2009) or by ecologists in general. *Ecology Letters* **13**:E7–E9
- Simpson & Birks (2012) *Statistical learning in palaeolimnology*. In Birks, H.J.B, Lotter, A.F. Juggins S., and Smol, J.P. (Eds) Tracking Environmental Change Using Lake Sediments, Volume 5: Data Handling and Numerical Techniques. Springer, Dordrecht.

Generalised Linear Models

- Generalised linear models (GLMs) are a synthesis and extension of linear regression plus Poisson, logistic and other regression models
- GLMs extend the types of data and error distributions that can be modelled beyond the Gaussian data of linear regression
- With GLMs we can model count data, binary/presence absence data, and concentration data where the response variable is not continuous.
- Such data have different mean-variance relationships and we would not expect errors to be Gaussian.
- Typical uses of GLMs in ecology are
  - Poisson GLM for count data
  - Logistic GLM for presence absence data
  - Gamma GLM for non-negative or positive continuous data
- GLMs can handle many problems that appear non-linear
- Not necessary to transform data as this is handled as part of the GLM process

Structure of a GLM

A GLM consists of three components, chosen/specified by the user

1. A random component, specifying the conditional distribution of of the response Y_i given the values of the explanatory data. Error Function
2. A Linear Predictor η — the linear function of regressors

   $$\eta_i = \alpha + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_k X_{ik}$$

   The X_{ij} are prescribed functions of the explanatory variables and can be transformed variables, dummy variables, polynomial terms, interactions etc.
3. A smooth and invertible Link Function $g(\cdot)$, which transforms the expectation of the response $\mu_i \equiv E(Y_i)$ to the linear predictor

   $$g(\mu_i) = \eta_i = \alpha + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_k X_{ik}$$

   As $g(\cdot)$ is invertible, we can write

   $$\mu_i = g^{-1}(\eta_i) = g^{-1}(\alpha + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_k X_{ik})$$

GLM Error Function

- Originally GLMs were specified for error distribution functions belonging to the exponential family of probability distributions
- Continuous probability distributions
  - Normal (linear regression)
  - Weibull
  - Gamma (data with constant coefficient of variation)
  - Exponential (time to death, survival analysis)
  - Chi-squared
  - Inverse-Gaussian
- Discrete probability distributions
  - Poisson (count data)
  - Binomial (0/1 data, proportions)
  - Multinomial
  - Hypergeometric
  - Pascal
- Choice depends on range of Y_i and on the relationship between the variance and the expectation of Y_i

GLM Error Function

Characteristics of common GLM probability distributions

Probability	Canonical Link	Range of Y_i	Variance function
Gaussian	Identity	$(-\infty, +\infty)$	ϕ
Poisson	Log	$0, 1, 2, \ldots, \infty$	μ_i
Binomial	Logit	$\frac{0,1,\ldots,n_i}{n_i}$	$\frac{\mu_i(1-\mu_i)}{n_i}$
Gamma	Inverse	$(0, \infty)$	$\phi\mu_i^2$
Inverse-Gaussian	Inverse-square	$(0, \infty)$	$\phi\mu_i^3$

ϕ is the dispersion parameter; μ_i is the expectation of Y_i. In the binomial family, n_i is the number of trials

Ecologically Error Function

Normal errors rarely adequate in ecology; GLMs offer ecologically meaningful alternatives

- Poisson — counts; integers, non-negative, variance increases with mean
- Binomial — observed proportions from a total; integers, non-negative, bounded at 0 and 1, variance largest at $\pi = 0.5$
- Binomial — presence absence data; discrete values, 0 and 1, models probability of success
- Gamma — concentrations; non-negative (strictly positive with log link) real values, variance increases with mean, many zero values and some high values

Logistic regression — Darlingtonia

- Timed censuses at 42 randomly-chosen leaves of the cobra lily (*Darlingtonia californica*)
- Recorded number of wasp visits at 10 of the 42 leaves
- Test hypothesis that the probability of visitation is related to leaf height
- Response is dichotomous variable (0/1)
- A suitable model is the logistic model

$$\pi = \frac{e^{\beta_0 + \beta_i X}}{1 + e^{\beta_0 + \beta_1 X_i}}$$

- The logit transformation produces

$$\log_e \left(\frac{\pi}{1 - \pi} \right) = \beta_0 + \beta_1 X_i$$

- This is the logistic regression and it is a special case of the GLM, with a binomial error distribution and the logit link function

Logistic regression — Darlingtonia

$$\log_e \left(\frac{\pi}{1 - \pi} \right) = \beta_0 + \beta_1 X_i$$

- β_0 is a type of intercept; determines the probability of success $(Y_i = 1)$ π where X = 0
- If $\beta_0 = 0$ then $\pi = 0.5$
- β_1 is similar to the slope and determines how steeply the fitted logistic curve rises to the maximum value of $\pi = 1$
- Together, β_0 and β_1 specify the range of the X variable over which most of the rise occurs and determine how quickly the probability rises from 0 to 1
- Estimate the model parameters using Maximum Likelihood; find parameter values that make the observed data most probable

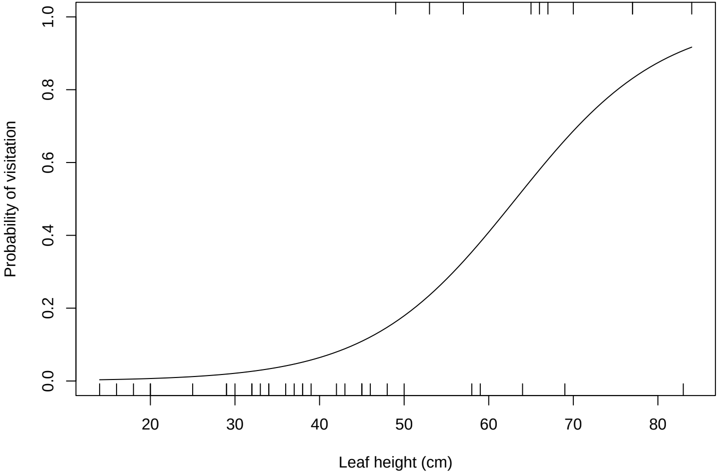
Logistic regression — Darlingtonia

```
> mod <- glm(visited ~ leafHeight, data = wasp, family = binomial)
> mod

Call:  glm(formula = visited ~ leafHeight, family = binomial, data = wasp)

Coefficients:
(Intercept)   leafHeight
    -7.2930       0.1154

Degrees of Freedom: 41 Total (i.e. Null);  40 Residual
Null Deviance:      46.11
Residual Deviance: 26.96    AIC: 30.96

> ilogit(coef(mod))
 (Intercept)   leafHeight
0.0006798556 0.5288181121
```

Logistic regression — Darlingtonia

```
> summary(mod)

Call:
glm(formula = visited ~ leafHeight, family = binomial, data = wasp)

Deviance Residuals: 
     Min        1Q    Median        3Q       Max  
-2.18274  -0.46820  -0.23897  -0.08519   1.90573  

Coefficients:
            Estimate Std. Error z value Pr(>|z|)    
(Intercept) -7.29295    2.16081  -3.375 0.000738 ***
leafHeight   0.11540    0.03655   3.158 0.001591 ** 
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 46.105  on 41  degrees of freedom
Residual deviance: 26.963  on 40  degrees of freedom
AIC: 30.963

Number of Fisher Scoring iterations: 6
```

Logistic regression — Darlingtonia



Wald statistics

- z values are Wald statistics, which under the null hypothesis follow a normal distribution
- Tests the null hypothesis that $\beta_i = 0$

$$z = \hat{\beta}_i / \mathrm{SE}(\hat{\beta}_i)$$

```
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -7.29295    2.16081  -3.375 0.000738 ***
leafHeight   0.11540    0.03655   3.158 0.001591 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Deviance

- In least squares we have the residual sum of squares as the measure of lack of fitted
- In GLMs, deviance plays the same role
- Deviance is defined as twice the log likelihood of the observed data under the current model
- Deviance is defined relative to an arbitrary constant — only differences of deviances have any meaning
- Differences in deviances are also known as ratios of likelihoods
- An alternative to the Wald tests are deviance ratio or likelihood ratio tests

$$F = \frac{(D_a - D_b)/(\mathrm{df}_a - \mathrm{df}_b)}{D_b/\mathrm{df}_b}$$

- D_j deviance of model, where we test if model A is a significant improvement over model B; df_k are the degrees of freedom of the respective model

A Gamma GLM — simple age-depth modelling

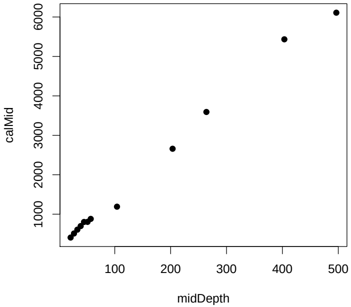
- Radiocarbon age estimates from depths within a peat bog (Brew & Maddy, 1995, QRA Technical Guide No. 5)
- Estimate accumulation rate; assumption here is linear accumulation
- Uncertainty or error is greater at depth; mean variance relationship
- Here, fit mid-depth & mid-calibrated age points

	upperDepth	lowerDepth	ageBP	ageError	calUpper	calLower
SRR-4556	20	22.00	355	35	509	307
SRR-4557	26	28.00	465	35	542	480
SRR-4558	32	34.00	635	35	671	545
SRR-4559	38	40.00	740	35	732	666
SRR-4560	44	46.00	865	35	916	691
SRR-4561	50	52.50	870	35	918	692
SRR-4562	56	58.00	985	35	967	795
SRR-4563	100	108.00	1270	35	1284	1097
SRR-4564	200	207.00	2575	35	2761	2558
SRR-4565	260	268.00	3370	35	3697	3487
SRR-4566	400	407.00	4675	35	5563	5306
SRR-4567	493	500.00	5315	35	6263	5955

A Gamma GLM — simple age-depth modelling

```
> plot(calMid ~ midDepth, data = peat,
+      pch = 21, bg = "black")
> m2 <- glm(calMid ~ midDepth, data = peat,
+           family = Gamma(link = "identity"))
> summary(m2)

Call:
glm(formula = calMid ~ midDepth,
    family = Gamma(link = "identity"), data = peat)

Deviance Residuals:
      Min         1Q     Median         3Q        Max
-0.196221  -0.012606  -0.001604   0.050645   0.092314

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 181.0393    26.0842   6.941 3.99e-05 ***
midDepth     12.2807     0.5025  24.441 3.00e-10 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for Gamma family taken to be 0.005924447)

    Null deviance: 10.439047  on 11  degrees of freedom
Residual deviance:  0.063394  on 10  degrees of freedom
AIC: 148.83

Number of Fisher Scoring iterations: 4
```

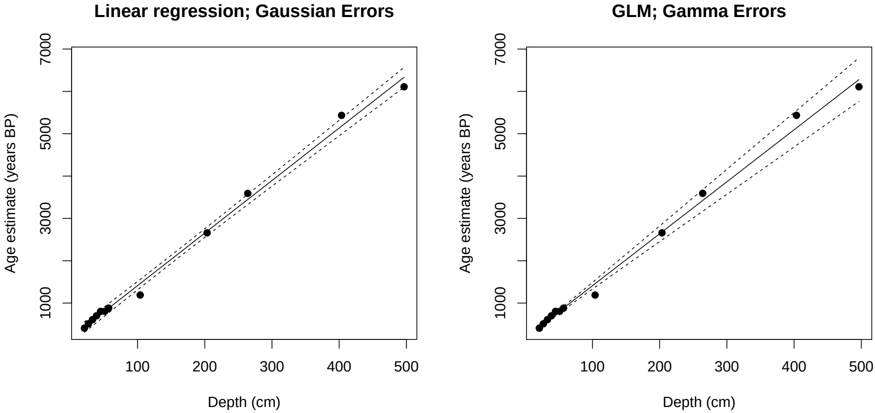
- Linear relationship
- Error increases with mean & Gamma errors
- Identity link function maintains linearity



A Gamma GLM — simple age-depth modelling

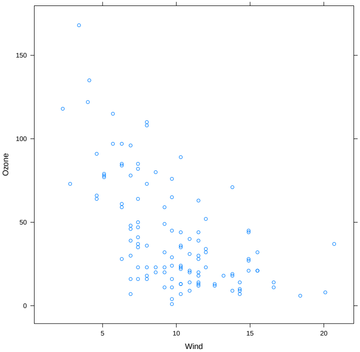
```
> anova(m2, test = "F")
Analysis of Deviance Table

Model: Gamma, link: identity

Response: calMid

Terms added sequentially (first to last)


         Df Deviance Resid. Df Resid. Dev      F    Pr(>F)
NULL                        11    10.4390
midDepth  1   10.376        10     0.0634 1751.3 1.455e-12 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

A Gamma GLM — simple age-depth modelling



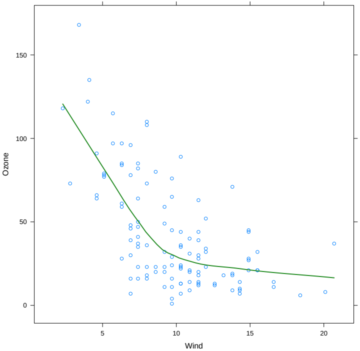
Scatterplots and local relationships

- In scatter plots, it is not always easy to see the form of the relationship between variables
- Ozone concentration tends to decrease as wind speed increases
- But it is difficult to judge whether this relationship is linear or non-linear



Scatterplots and local relationships

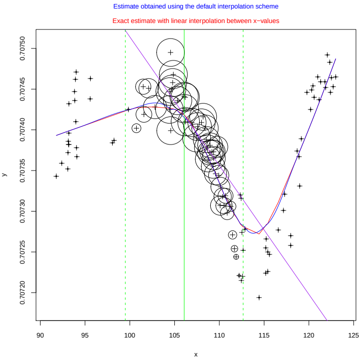
- In scatter plots, it is not always easy to see the form of the relationship between variables
- Ozone concentration tends to decrease as wind speed increases
- But it is difficult to judge whether this relationship is linear or non-linear
- Smoothers model the local patterns in a bivariate scatter plot to illustrate the trends or patterns in the data
- They determine the pattern from the data themselves rather than from an *a priori* defined model
- Loess (or Lowess) is one such smoothing technique



Lowess — Locally weighted regression

Locally weighted regression scatterplot smoother

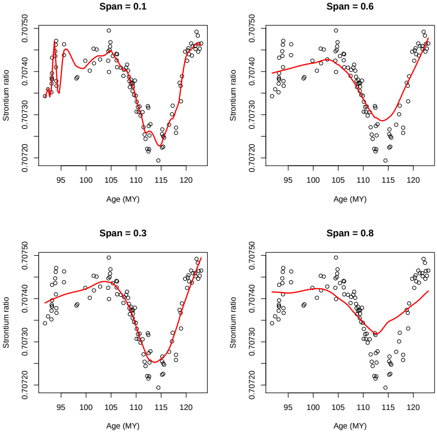
- Decide how smooth relationship should be (span or size of bandwidth window)
- For target point assign weights to observations based on adjacency to target point
- Fit linear (polynomial) regression to predict target using weighted least squares; repeat
- Compute residuals & estimate robustness weights based on residuals; well-fitted points have high weight
- Repeat Loess procedure with new weights based on robustness and distance weights



Try different span and degree of polynomial to optimise fit

Lowess — Locally weighted regression

- Two key choices in Loess
- α is the span or bandwidth parameter, controls the size of the window about the target observation
- Observation outside the window have 0 weight
- Larger the window the more global the fit — smooth
- The smaller the window the more local the fit — rough
- λ is the degree of polynomial using the the weighted least squares
- $\lambda = 1$ is a linear fit, $\lambda = 2$ is a quadratic fit



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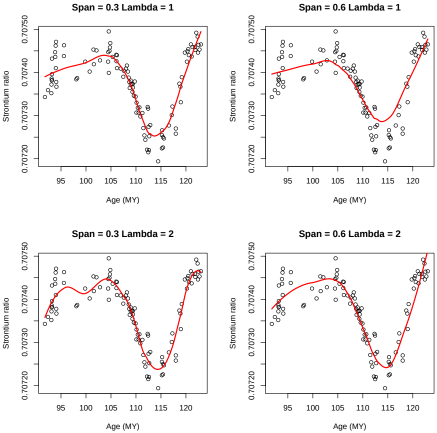


Lowess — Locally weighted regression

"In any specific application of LOESS, the choice of the two parameters α and λ must be based upon a combination of judgement and trial and error. There is no substitute for the latter"

Cleveland (1993) Visualising Data. AT&T Bell Laboratories

- CV can be used to optimise α and λ to guard against overfitting the local pattern by producing too rough a smoother or missing local pattern by producing too smooth a smoother
- However, there are techniques with better properties such as splines that have fewer parameters to choose and which are more widely used
- Loess is perhaps most useful as an exploratory technique as part of EDA
- Cleveland, W.S. (1979) J. Amer. Stat. Assoc. **74**, 829–836
- Cleveland, W.S. (1994) The Elements of Graphing Data. AT&T Bell Laboratories
- Efron, B & Tibshirani, R (1981) Science **253**, 390–395

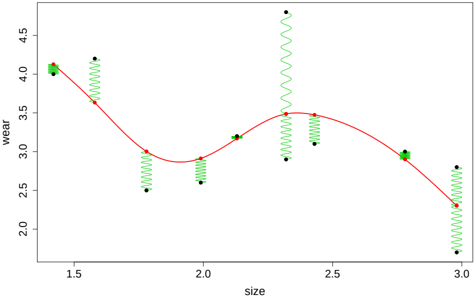
Splines

- Splines are mathematical functions that take their name from the flexible strips of materials draughtsmen used to draw curves
- A simple spline would just connect the dots, joining each observation to the next — minimal error but rough
- Impose a penalty (λ) on the degree of roughness, so fitting the spline balances the error (lack of fit to the data) with the complexity (roughness) of the spline — smoothing spline
- Smoothing splines useful alternative to Lowess for EDA and scatterplot smoothing
- Smoothing splines consist of a series of cubic polynomials over intervals of the data, with intervals defined by knots — piecewise cubic polynomial which is continuous as are it's first a second derivatives

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3$$

Splines

- All the smooths covered here are based on *splines*. Here's the basic idea . . .



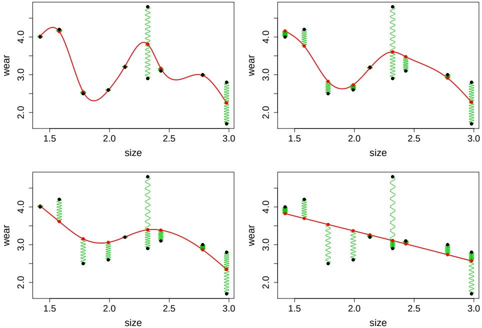
- Mathematically the red curve is the *function* minimizing

$$\sum_i (y_i - f(x_i))^2 + \lambda \int f''(x)^2 dx.$$

Source: Simon Wood

Splines have variable stiffness

- Varying the flexibility of the strip (i.e. varying λ) changes the *spline function* curve.



- But irrespective of λ the spline functions always have the same basis.

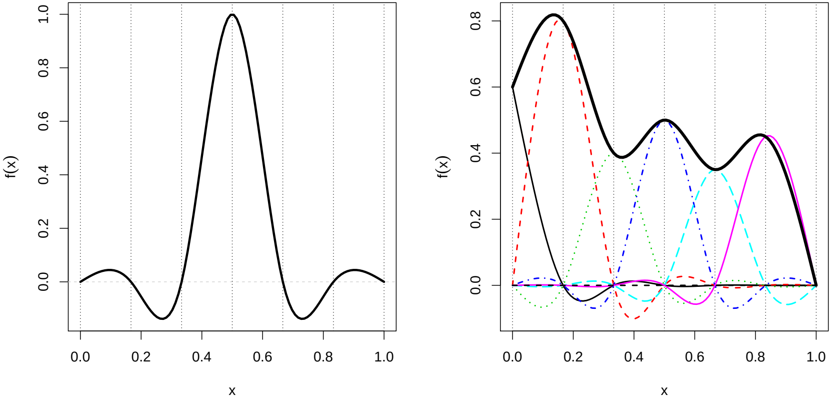
Source: Simon Wood

Splines

- Regression splines are an alternative type of spline more commonly found in statistical techniques (GAMs)
- In smoothing splines, the observations are the knots and the smoothness is controlled by roughness penalty λ
- In regression splines, a smaller set of knots is chosen across range of the data and cubic polynomials are fitted to the intervals defined by the knots
- As a result, in regression splines the number of knots controls the smoothness of the fitted function
- Once the knots are chosen, regression splines are arguably a parametric approach as we only need to determine the coefficients for the parametric cubic polynomials fitted to each interval
- Regression splines more closely link with formal statistical modelling — can include spline terms in linear regression models and use least squares to estimate parameters

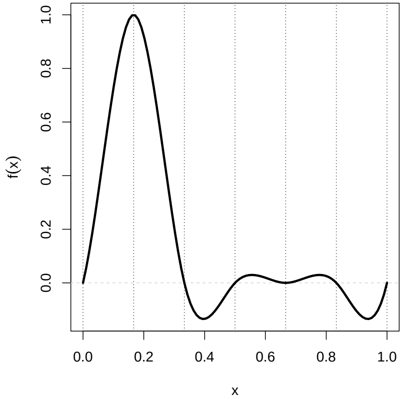
Basis functions — cubic regression splines

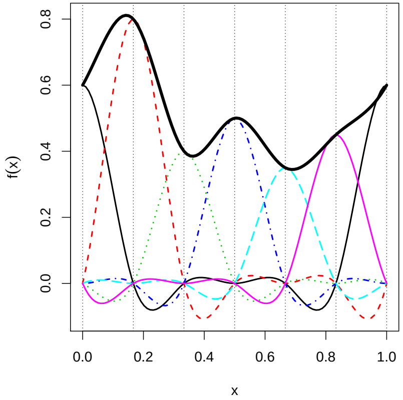
- Cubic regression spline basis function takes value 1 at one knot and 0 at others
- jth basis function is multiplied by it's coefficient β_j and then each of these curves is summed at the values of x to yield the smooth curve



Basis functions — cyclic cubic regression splines

- Where x represents a cyclic variable, want ends points of spline to join up smoothly
- Additional constraints on basis functions; second derivatives must match at $f(x_1)$ and $f(x_k)$ (i.e. knots at end points)





Generalised Additive Models

- Generalised Additive Models (GAMs) are a semi-parametric extension of the GLM

$$g(\mu_i) = \eta_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \cdots + \beta_k x_{ki}$$

- GLM requires an *a priori* statistical model
- What if the response can not be well modelled using the available model forms?
- Despite their flexibility, GLMs may not be flexible enough to approximate the true response adequately
- GLMs are model driven
- GAMs include smooth terms of one or more predictors rather than parametric terms
- The form of the smoothers is derived from the data — GAMs are data driven

Generalised Additive Models

- Generalised Additive Models (GAMs) for a single covariate has the form

$$g(\mu_i) = \eta_i = \beta_0 + f_1(x_{1i})$$

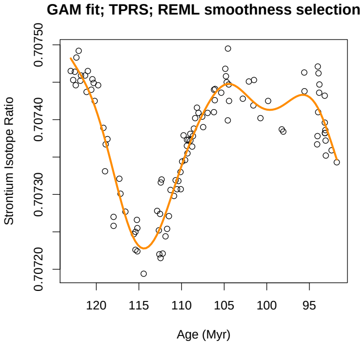
- The models are additive as all we assume is that the model terms combine in an additive manner to produce the fitted values of the response
- A GAM consisting of smooth terms for several variables has the form

$$g(\mu_i) = \eta_i = \beta_0 + f_1(x_{1i}) + f_2(x_{2i}) + \cdots f_k(x_{ki}) = \beta_0 + \sum_{k=1}^{m} f_k(x_{ki})$$

- The smooth functions can one of many types of smoother — splines
- Need to specify the type of smoother and complexity of each smoother
- The degree of smoothing for each smooth term can be estimated as part of the model fitting

GAM — Strontium isotope ratios

```
> require(mgcv)
> m <- gam(strontium.ratio ~ s(age), data = fossil,
+          method = "REML")
> summary(m)

Family: gaussian
Link function: identity

Formula:
strontium.ratio ~ s(age)

Parametric coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 7.074e-01  2.551e-06  277241   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Approximate significance of smooth terms:
         edf Ref.df  F p-value
s(age) 8.244   8.84 88  <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

R-sq.(adj) =  0.881   Deviance explained =   89%
REML score = -930.01  Scale est. = 6.9006e-10  n = 106
```



Generalised Additive Models

- In all other respects, GAMs are just like GLMs (link functions, error distributions, etc)
- Using modern methods, the degree of smoothing can be determined alongside the other model parameters using ML
- Interactions can be modelled using a smooth function of two or more variables

$$g(\mu_i) = \eta_i = \beta_0 + f_1(x_{1i}, x_{2i})$$

- In above, thin plate splines impose same degree of smoothing on both variables, tensor product smooths allow for different amounts of smoothing
- Cyclic variables may be modelled using a cyclic smoother; the end points of the smoother are forced to match with no discontinuity

Selected texts

- Wood, S.N. (2006) Generalised additive models; and introduction with R. Chapman & Hall/CRC
- Ruppert, Wand, & Carroll (2003) Semiparametric regression. Cambridge University Press
- Faraway (2006) Extending the linear model with R; generalized linear, mixed effects and nonparametric regression models. Chapman & Hall/CRC
- Zuur, Ieno, Walker, Saveliev, & Smith (2009) Mixed effects models and extensions in ecology with R. Springer

Miscellaneous R commands for working with models

- It is recommended to use extractor functions for the model object
- Common extractor and utility functions are:
    - `coef()`: model coefficients
    - `fitted()`: fitted values
    - `resid()`: model residuals
    - `vcov()`: variance-covariance matrix of main model parameters
    - `predict()`: predict from model
    - `extractAIC()`, `AIC()`: AIC of model
    - `logLik()`: log likelihood of fitted model
    - `print()`: quick textual display of object
    - `summary()`: longer textual display of object
    - `plot()`: plot the model diagnostics
    - `add1()`, `drop1()`: add/delete single terms
    - `update()`: refit the model with changes to formula
    - `anova()`: partition variance amongst terms or compare models