Statistical Models in S

The template is a multiple linear regression model:

$$y_i = \sum_{j=1}^{p} x_{ij}\beta_j + e_i \text{ where } e_i \sim \text{NID}(0, \sigma^2)$$

In matrix terms this would be written

$$y = X\beta + e$$

where

- $\boldsymbol{y}$ is the response vector,
- $\boldsymbol{\beta}$ is the vector of regression coefficients,
- $\mathbf{X}$ is the *model matrix* or *design matrix* and
- $\boldsymbol{e}$ is the error vector.

Model formulae

General form: *yvar ~ term1 + term2 + ...*

Examples:

```
y ~ x                          – Simple regression
y ~ 1 + x                      – Explicit intercept
y ~ -1 + x                     – Through the origin
y ~ x +x^2                     – Quadratic regression
y ~ x1 + x2 + x3               – Multiple regression
y ~ G + x1 + x2                – Parallel regressions
y ~ G/(x1 + x2)                – Separate regressions
sqrt(Hard) ~ Dens+Dens^2       – Transformed
```

More examples of formulae

`y ~ G`	– Single classification
`y ~ A + B`	– Randomized block
`y ~ B + N*P`	– Factorial in blocks
`y ~ x + B + N*P`	– with covariate
`y ~ . - X1`	– All variables except `X1`
`. ~ . + A:B`	– Add interaction (update)
`Nitrogen ~ Times*(River/Site)`	- more complex design

Generic functions for inference

The following apply to most modelling objects

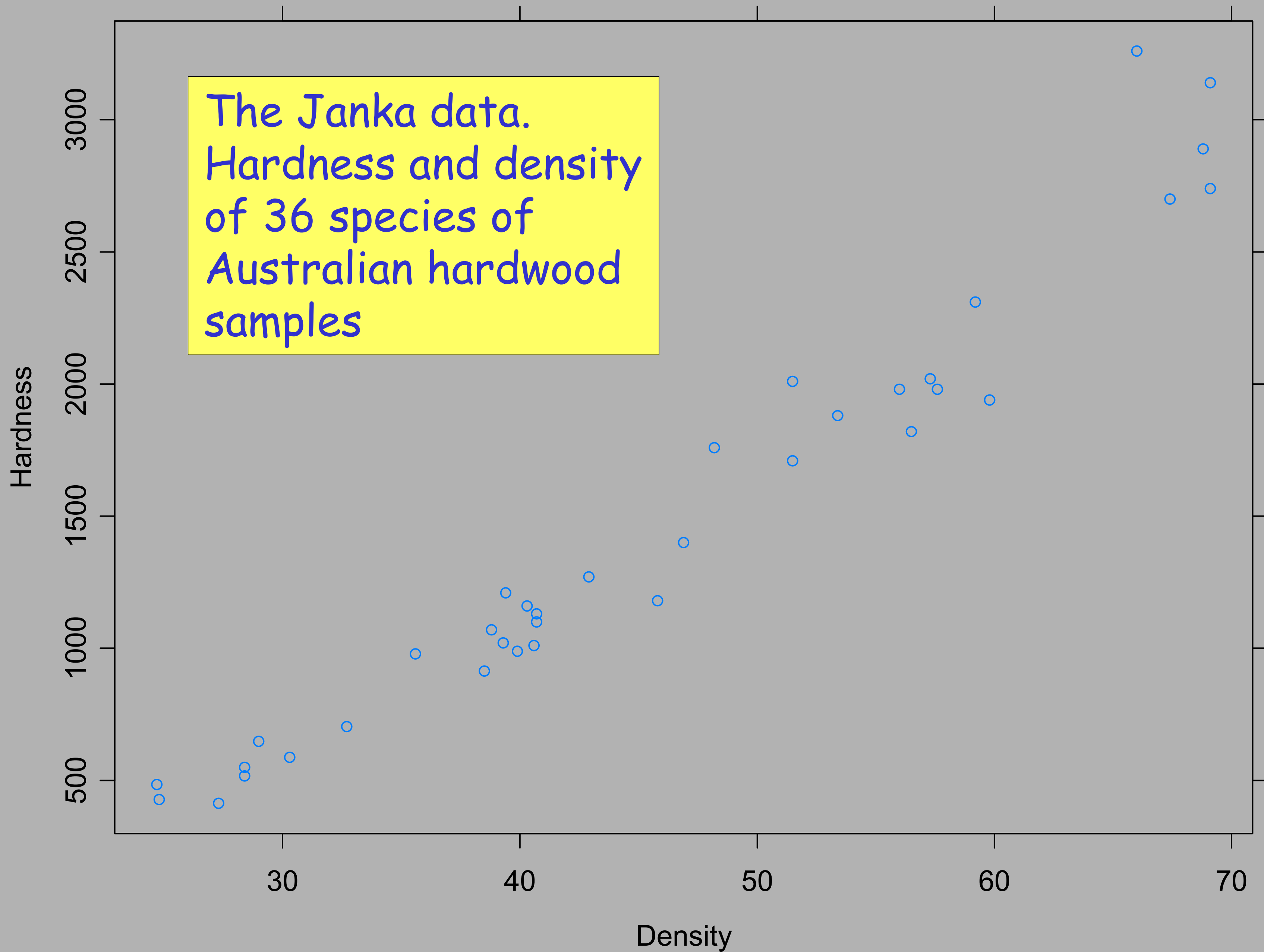
`coef(obj)`	regression coefficients
`resid(obj)`	residuals
`fitted(obj)`	fitted values
`summary(obj)`	analysis summary
`predict(obj,newdata = ndat)`	predict for new data
`deviance(obj)`	residual sum of squares

Example: The Janka data

Hardness and density data for 36 samples of Australian hardwoods.

Source: E. J. Williams, “Regression Analysis”, Wiley, 1959. [ex-CSIRO, Forestry.]

Problem: build a prediction model for Hardness using Density.


The Janka data.
Hardness and density of 36 species of Australian hardwood samples
Hardness
500
1000
1500
2000
2500
3000
30
40
50
60
70
Density

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Janka data - initial model building

We might start with a linear or quadratic model (suggested by Williams) and start checking the fit.

```
> jank.1 <- lm(Hard ~ Dens, janka)
> jank.2 <- update(jank.1, . ~ . + Dens^2)
> summary(jank.2)$coef
                Value Std. Error t value Pr(>|t|)
(Intercept) -118.00738 334.96690 -0.35230 0.726857
Dens           9.43402  14.93562  0.63165 0.531970
I(Dens^2)      0.50908   0.15672  3.24830 0.002669
```

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Janka data: a cubic model?

To check for the need for a cubic term we simply add one more term to the model

```
> jank.3 <- update(jank.2, . ~ . + Dens^3)
> summary(jank.3)$coef
                  Value Std. Error t value Pr(>|t|)
(Intercept) -6.4144e+02 1.2357e+03 -0.51911 0.60726
Dens         4.6864e+01 8.6302e+01  0.54302 0.59088
I(Dens^2)   -3.3117e-01 1.9140e+00 -0.17303 0.86372
I(Dens^3)    5.9587e-03 1.3526e-02  0.44052 0.66252
```

A quadratic term is necessary, but a cubic is not supported.

Janka data - stability of coefficients

The regression coefficients should remain more stable under extensions to the model if we standardize, or even just mean-correct, the predictors:

```
> janka$d <- scale(janka$Dens, scale=F)
> jank.1 <- lm(Hard ~ d, janka)
> jank.2 <- update(jank.1, .~.+d^2)
> jank.3 <- update(jank.2, .~.+d^3)
```

```
summary(jank.1)$coef
                  Value Std. Error t value Pr(>|t|)
(Intercept) 1469.472    30.5099  48.164        0
          d   57.507     2.2785  25.238        0
> summary(jank.2)$coef
                    Value Std. Error t value Pr(>|t|)
(Intercept) 1378.19661   38.93951 35.3933 0.000000
          d   55.99764    2.06614 27.1026 0.000000
     I(d^2)    0.50908    0.15672  3.2483 0.002669
> round(summary(jank.3)$coef, 4)
                   Value Std. Error t value Pr(>|t|)
(Intercept) 1379.1028    39.4775 34.9339   0.0000
          d   53.9610     5.0746 10.6336   0.0000
     I(d^2)    0.4864     0.1668  2.9151   0.0064
     I(d^3)    0.0060     0.0135  0.4405   0.6625
```

Why is this so? Does it matter very much?

Checks and balances

```
> xyplot(studres(janka.lm2) ~ fitted(janka.lm2),
   panel = function(x, y, ...) {
      panel.xyplot(x, y, col = 5, ...)
      panel.abline(h = 0, lty = 4, col = 6)
   }, xlab = "Fitted values", ylab = "Residuals")
> qqmath(~ studres(janka.lm2), panel =
   function(x, y, ...) {
        panel.qqmath(x, y, col = 5, ...)
        panel.qqmathline(y, qnorm, col = 4)
     }, xlab = "Normal scores",
     ylab = "Sorted studentized residuals")
```

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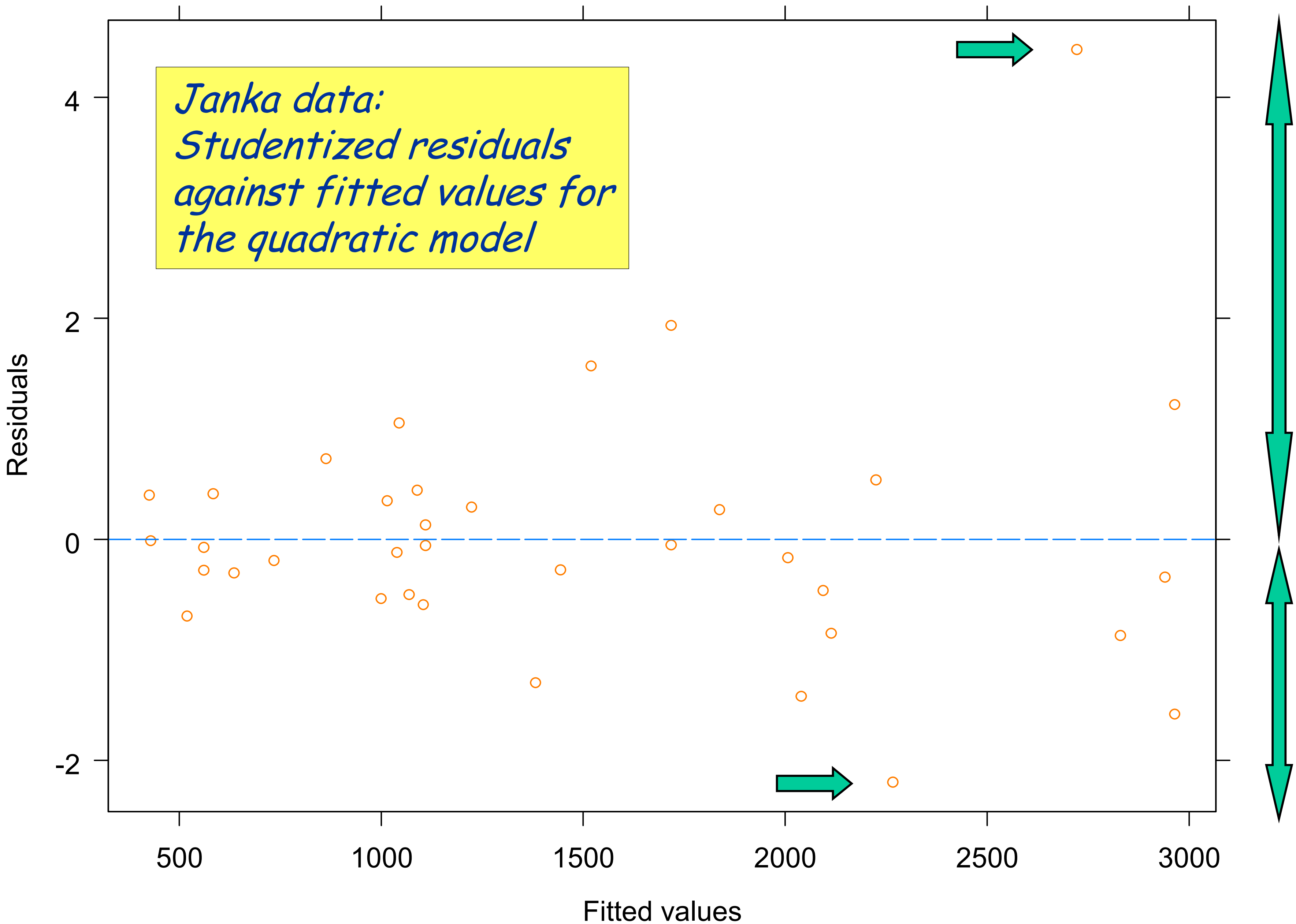

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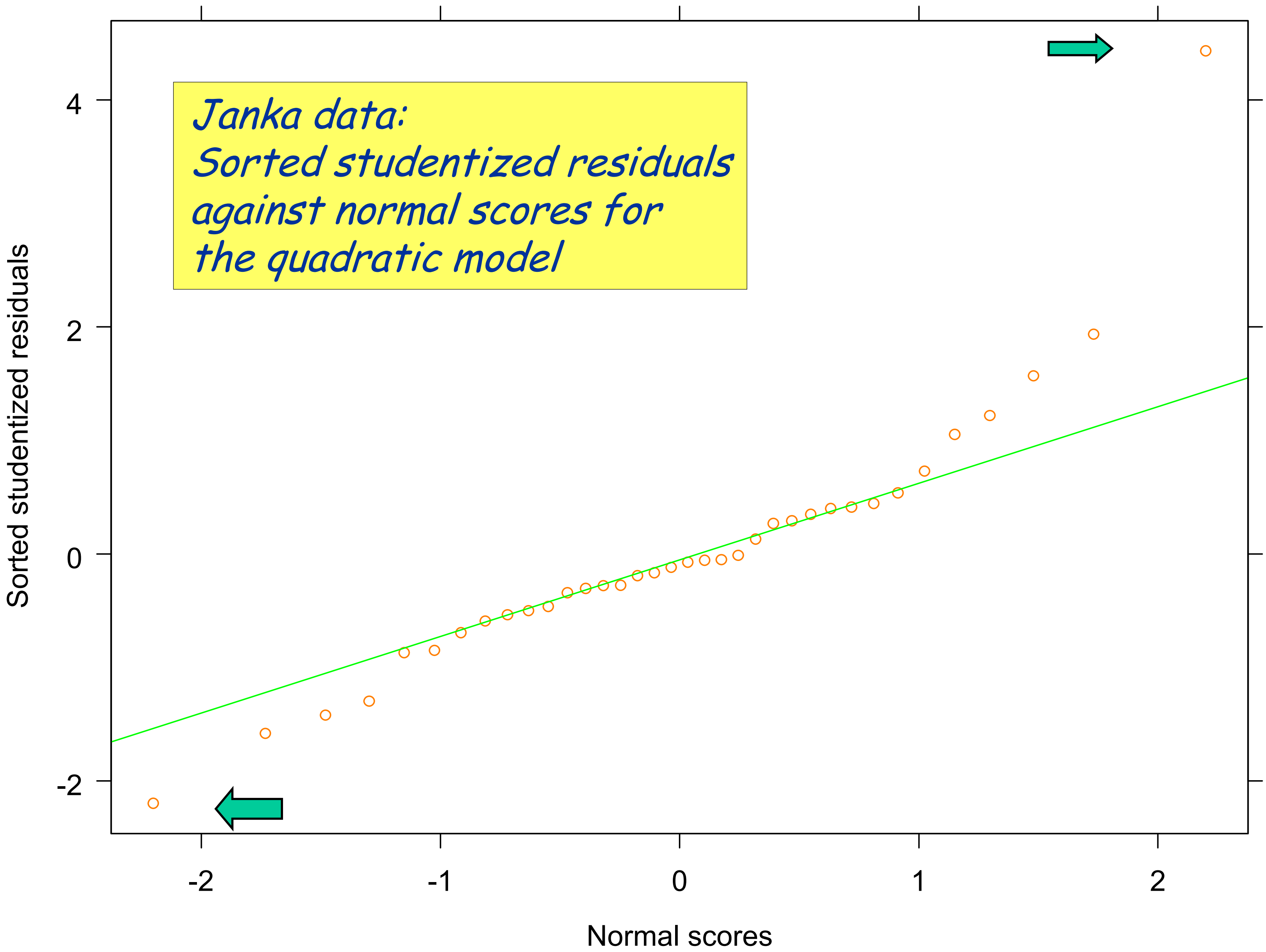

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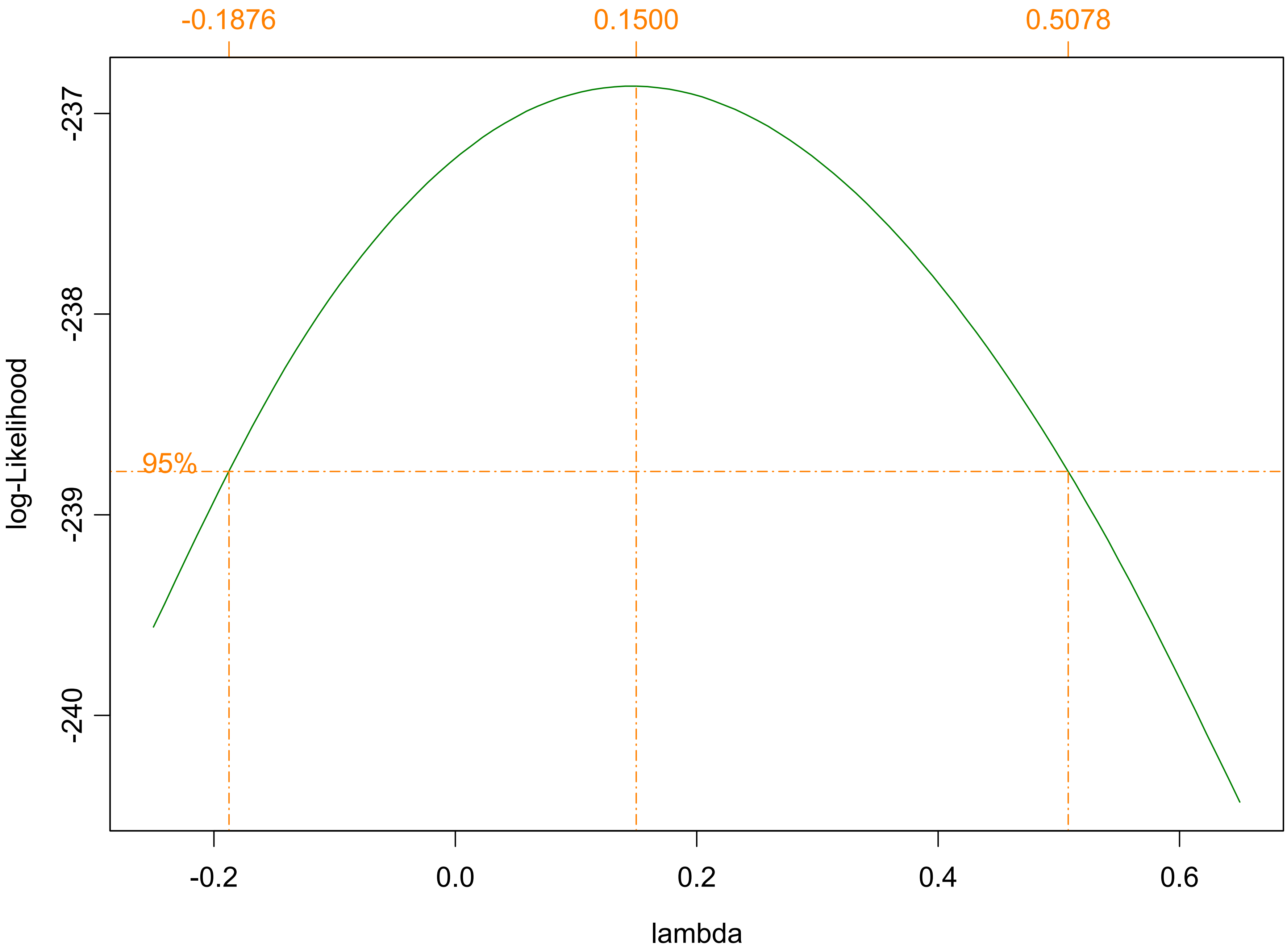
Janka data - trying a transformation

The Box-Cox family of transformations includes square-root and log transformations as special cases.

The `boxcox` function in the MASS library allows the marginal likelihood function for the transformation parameter to be calculated and displayed. It's use is easy. (Note: it only applies to *positive* response variables.)

```
> library(MASS, first = T)
> graphsheet() # necessary if no graphics device open.
> boxcox(jank.2,
         lambda = seq(-0.25, 1, len=20))
```



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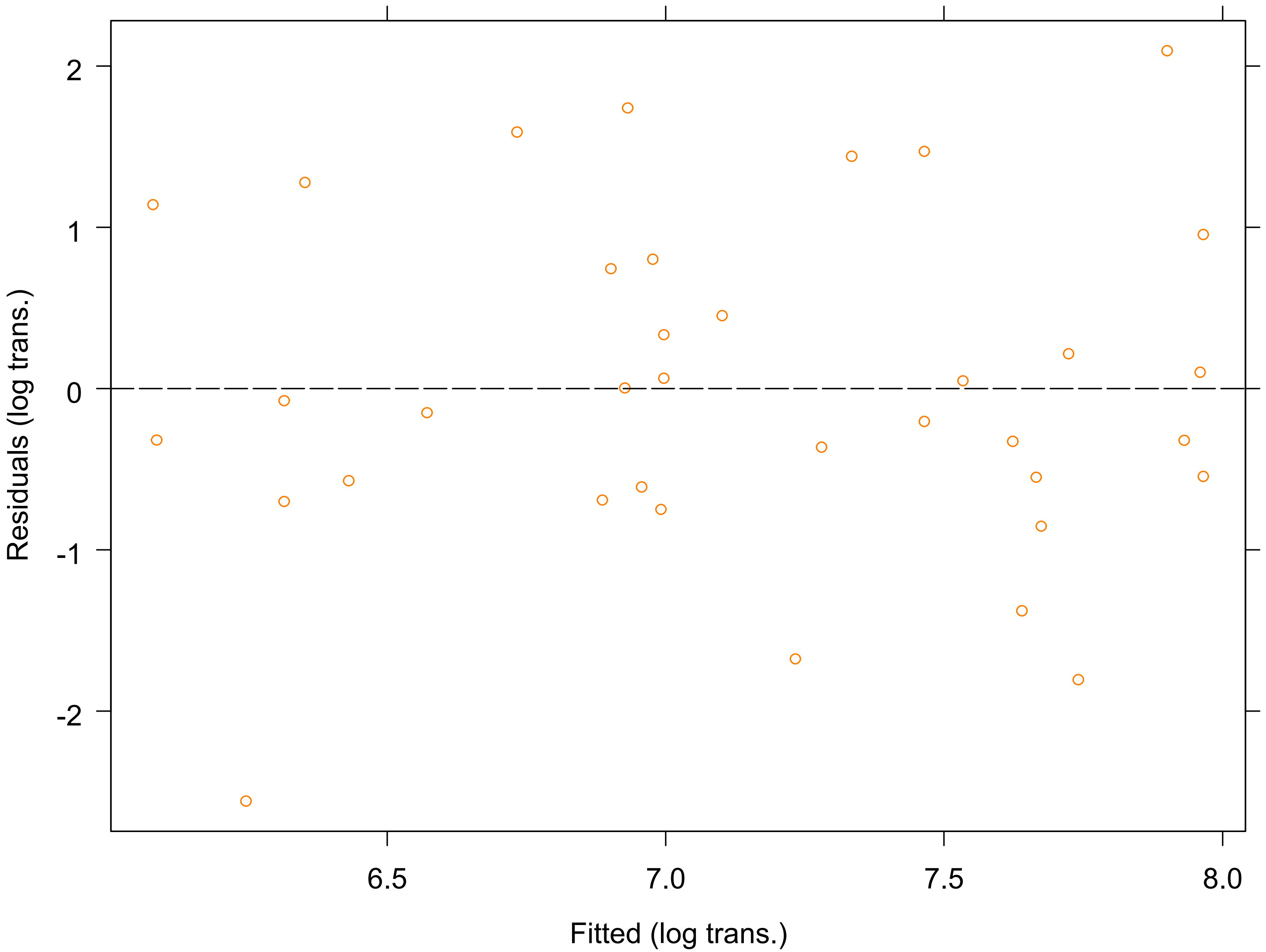
Janka data - transformed data

The marginal likelihood plot suggests a log transformation.

```
> ljank.2 <- update(jank.2, log(.)˜.)
> round(summary(ljank.2)$coef, 4)
              Value Std. Error   t value Pr(>|t|)
(Intercept)  7.2299     0.0243  298.0154        0
          d  0.0437     0.0013   33.9468        0
     I(d^2) -0.0005     0.0001   -5.3542        0
> lrs <- studres(ljank.2)
> lfv <- fitted(ljank.2)
> xyplot(lrs ~ lfv, panel =
    function(x, y, ...) {
        panel.xyplot(x, y, ...)
        panel.abline(h=0, lty=4)
    }, xlab = "Fitted (log trans.)",
    ylab = "Residuals (log trans.)", col = 5)
```



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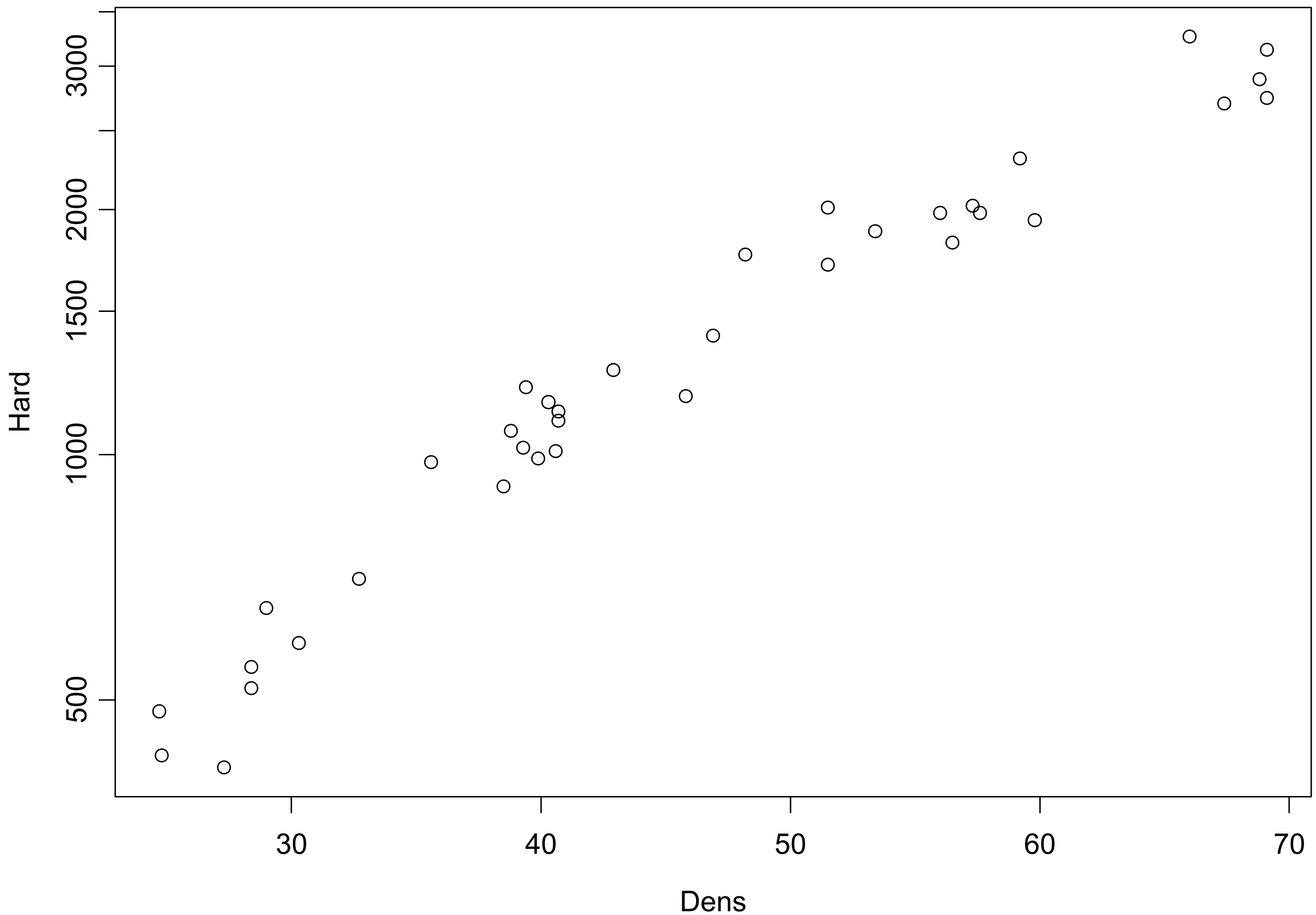
Plot of transformed data

```
> attach(janka)
> plot(Dens, Hard, log = "y")
```



Selecting terms in a multiple regression

Example: The Iowa wheat data.

```
> names(iowheat)
 [1] "Year"   "Rain0" "Temp1" "Rain1" "Temp2"
 [6] "Rain2" "Temp3" "Rain3" "Temp4" "Yield"
> bigm <- lm(Yield ~ ., data = iowheat)
```

fits a regression model using *all other variables* in the data frame as predictors.

From the big model, now check the effect of dropping each term individually:

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```
> dropterm(bigm, test = "F")
Single term deletions

Model:
Yield ~ Year + Rain0 + Temp1 + Rain1 + Temp2 + Rain2 +
  Temp3 + Rain3 + Temp4
       Df Sum of Sq    RSS    AIC F Value   Pr(F)
<none>                1404.8 143.79
  Year  1    1326.4 2731.2 163.73  21.715 0.00011
 Rain0  1     203.6 1608.4 146.25   3.333 0.08092
 Temp1  1      70.2 1475.0 143.40   1.149 0.29495
 Rain1  1      33.2 1438.0 142.56   0.543 0.46869
 Temp2  1      43.2 1448.0 142.79   0.707 0.40905
 Rain2  1     209.2 1614.0 146.37   3.425 0.07710
 Temp3  1       0.3 1405.1 141.80   0.005 0.94652
 Rain3  1       9.5 1414.4 142.01   0.156 0.69655
 Temp4  1      58.6 1463.5 143.14   0.960 0.33738
```

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```
> smallm <- update(bigm, . ~ Year)
> addterm(smallm, bigm, test = "F")
Single term additions

Model:
Yield ~ Year
       Df Sum of Sq    RSS    AIC F Value    Pr(F)
<none>               2429.8 145.87
 Rain0  1    138.65 2291.1 145.93  1.8155 0.18793
 Temp1  1     30.52 2399.3 147.45  0.3816 0.54141
 Rain1  1     47.88 2381.9 147.21  0.6031 0.44349
 Temp2  1     16.45 2413.3 147.64  0.2045 0.65437
 Rain2  1    518.88 1910.9 139.94  8.1461 0.00775
 Temp3  1    229.14 2200.6 144.60  3.1238 0.08733
 Rain3  1    149.78 2280.0 145.77  1.9708 0.17063
 Temp4  1    445.11 1984.7 141.19  6.7282 0.01454
```

Automated selection of variables

```
> stepm <- stepAIC(bigm,
            scope = list(lower = ~ Year))
Start:  AIC= 143.79
....
Step:  AIC= 137.13
 Yield ~ Year + Rain0 + Rain2 + Temp4

        Df Sum of Sq    RSS    AIC
 <none> NA        NA 1554.6 137.13
- Temp4  1    187.95 1742.6 138.90
- Rain0  1    196.01 1750.6 139.05
- Rain2  1    240.20 1794.8 139.87
>
```

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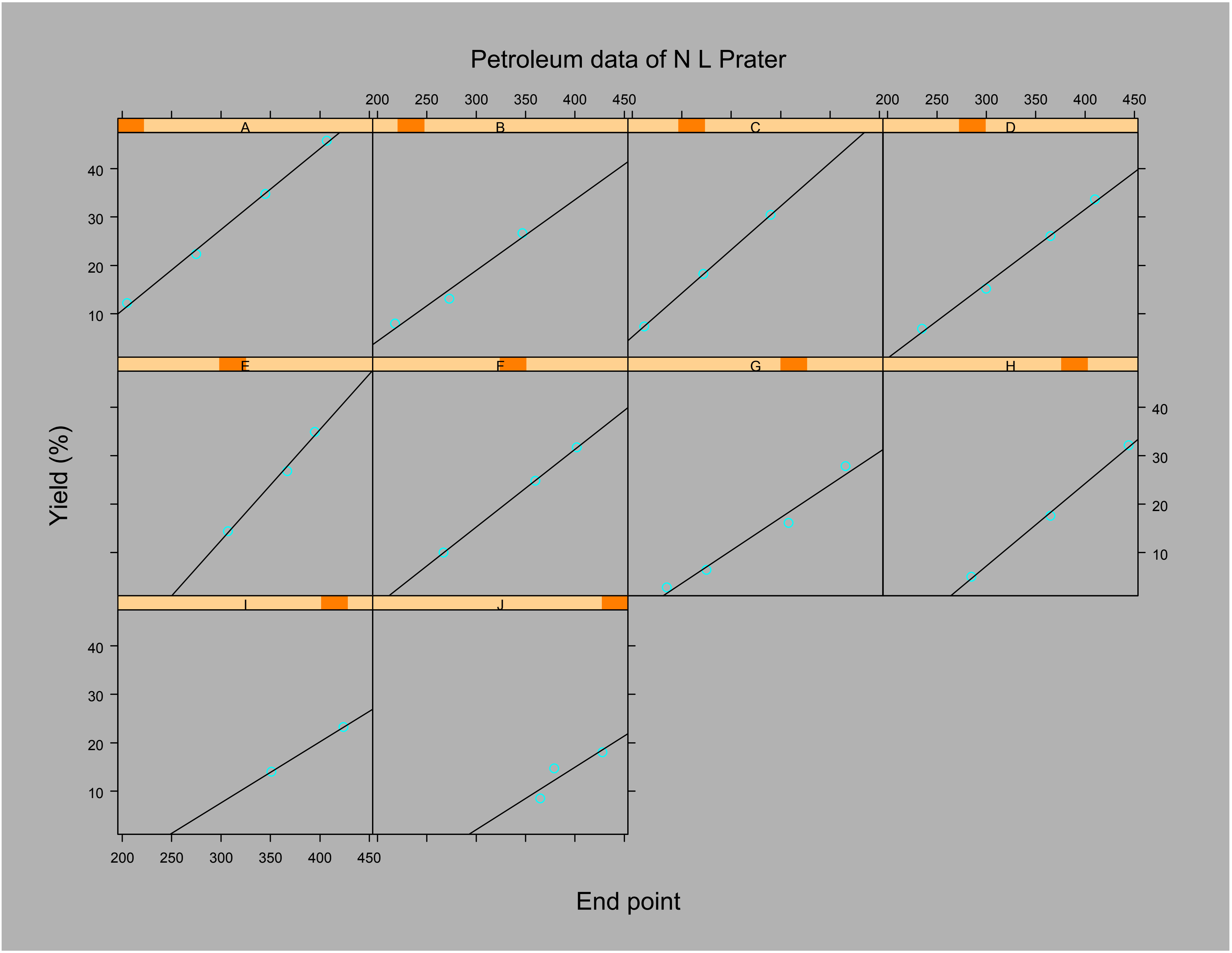
A Random Effects model

- The petroleum data of Nilon L Prater, (c. 1954).
- 10 crude oil sources, with measurements on the crude oil itself.
- Subsamples of crude (3-5) refined to a certain end point (measured).
- The response is the yield of refined petroleum (as a percentage).
- How can petroleum yield be predicted from properties of crude and end point?

A first look: Trellis display

For this kind of grouped data a Trellis display, by group, with a simple model fitted within each group is often very revealing.

```
> names(petrol)
[1] "No"  "SG"  "VP"  "V10" "EP"  "Y"
> xyplot(Y ~ EP | No, petrol, as.table = T,
    panel = function(x, y, ...) {
      panel.xyplot(x, y, ...)
      panel.lmline(x, y, ...)
    }, xlab = "End point", ylab = "Yield (%)",
    main = "Petroleum data of N L Prater")
>
```


Petroleum data of N L Prater
A
B
C
D
E
F
G
H
I
J
Yield (%)
End point
10
20
30
40
200
250
300
350
400
450

Fixed effect Models

Clearly a straight line model is reasonable.

There is some variation between groups, but parallel lines is also a reasonable simplification.

There appears to be considerable variation between intercepts, though.

```
> pet.2 <- aov(Y ~ No*EP, petrol)
> pet.1 <- update(pet.2, .~.-No:EP)
> pet.0 <- update(pet.1, .~.-No)
> anova(pet.0, pet.1, pet.2)
Analysis of Variance Table

Response: Y

    Terms Resid. Df    RSS   Test Df Sum of Sq F Value  Pr(F)
1      EP        30 1759.7
2 No + EP        21   74.1    +No  9    1685.6  74.101 0.0000
3 No * EP        12   30.3 +No:EP  9      43.8   1.926 0.1439
```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Random effects

```
> pet.re1 <- lme(Y ~ EP, petrol, random = ~1+EP|No)
> summary(pet.re1)
.....
     AIC    BIC   logLik
  184.77 193.18 -86.387

Random effects:
 Formula:  ~ 1 + EP | No
 Structure: General positive-definite
              StdDev   Corr
(Intercept) 4.823890 (Inter
         EP 0.010143 1
   Residual 1.778504

Fixed effects: Y ~ EP
              Value Std.Error DF t-value p-value
(Intercept) -31.990    2.3617 21 -13.545  <.0001
         EP   0.155    0.0062 21  24.848  <.0001
 Correlation:
   .....
```


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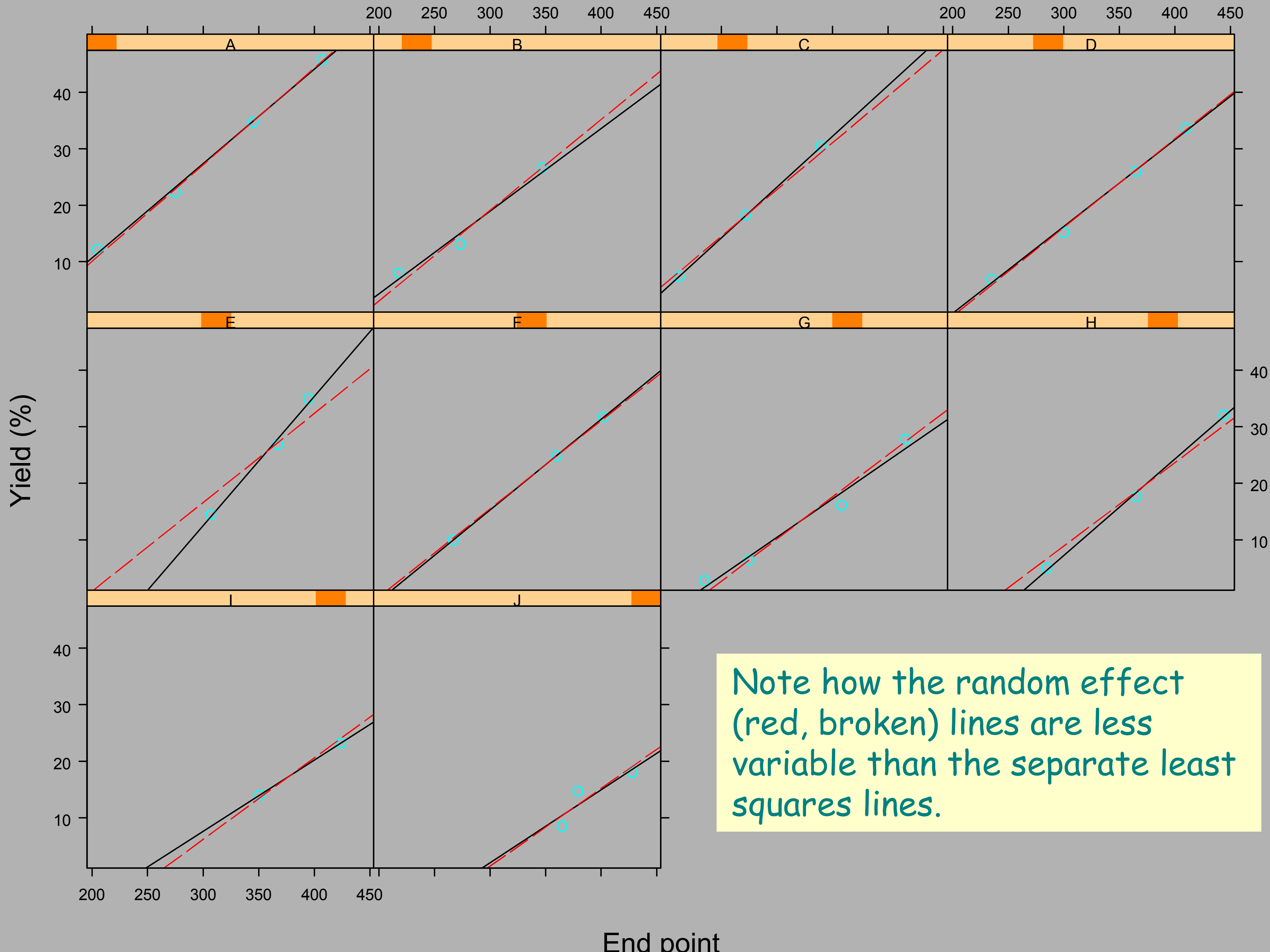
The shrinkage effect

```
> B <- coef(pet.re1)
> B
  (Intercept)       EP
A      -24.146 0.17103
B      -29.101 0.16062
C      -26.847 0.16536
D      -30.945 0.15674
E      -30.636 0.15739
F      -31.323 0.15595
G      -34.601 0.14905
H      -35.348 0.14748
I      -37.023 0.14396
J      -39.930 0.13785
> xyplot(Y ~ EP | No, petrol, as.table = T, subscripts = T,
    panel = function(x, y, subscripts, ...) {
        panel.xyplot(x, y, ...)
        panel.lmline(x, y, ...)
        wh <- as(petrol$No[subscripts][1], "character")
        panel.abline(B[wh, 1], B[wh, 2], lty = 4, col = 8)
    }, xlab = "End point", ylab = "Yield (%)")
```



Note how the random effect (red, broken) lines are less variable than the separate least squares lines.

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General notes on modelling

1. Analysis of variance models are linear models but usually fitted using `aov` rather than `lm`. The computation is the same but the resulting object behaves differently in response to some generics, especially `summary`.
2. Generalized linear modelling (logistic regression, log-linear models, quasi-likelihood, &c) also use *linear modelling formulae* in that they specify the model matrix, not the parameters. Generalized additive modelling (smoothing splines, loess models, &c) formulae are quite similar.
3. Non-linear regression uses a formula, but a completely different paradigm: the formula gives the full model as an expression, including parameters.

GLMs and GAMs: An introduction

- One generalization of multiple linear regression.
- Response, y, stimulus variables $x_1, x_2, \ldots, x_p$
- The distribution of Y depends on the x's through a single linear function, the 'linear predictor'

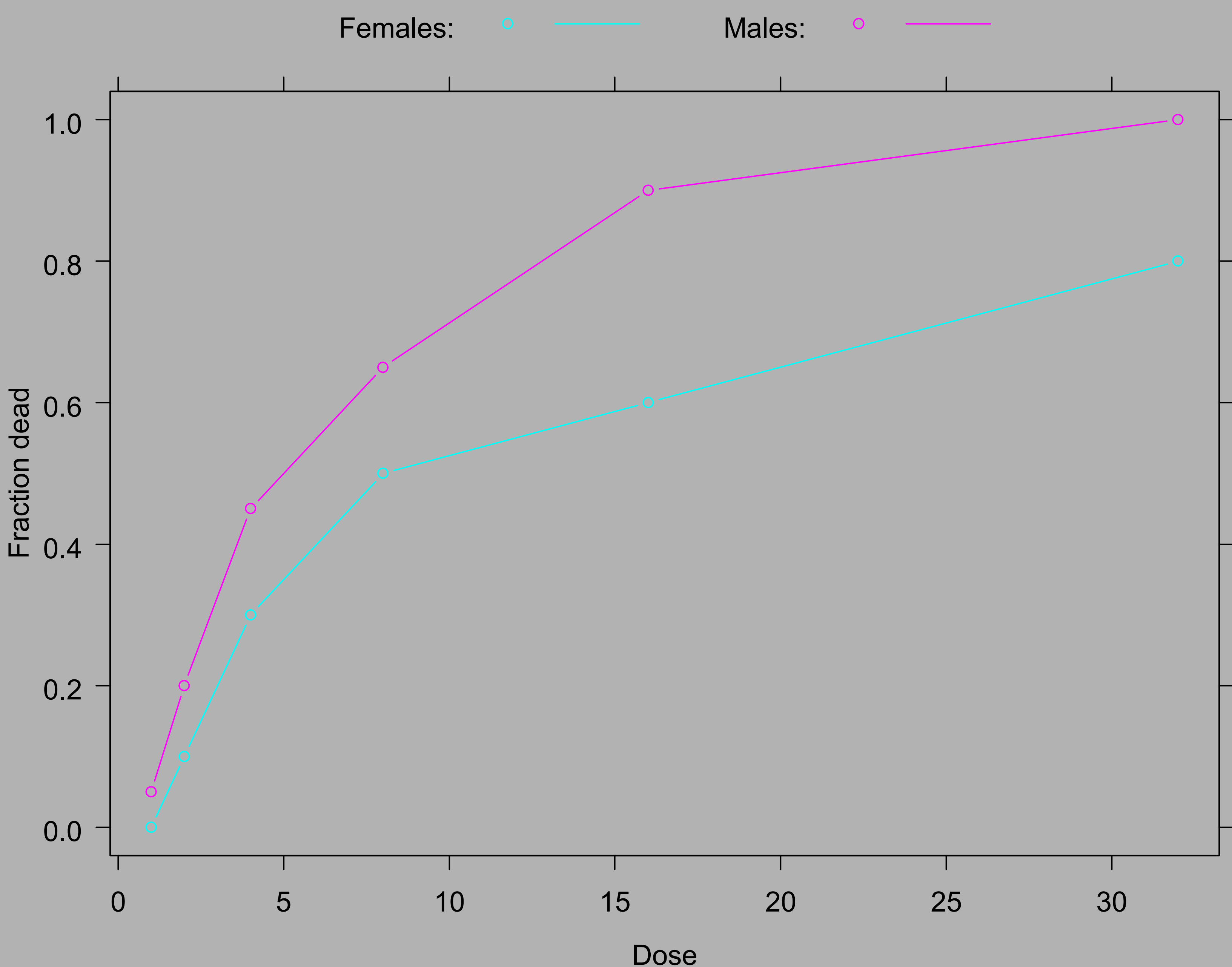
$$\eta = \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p$$

- There may be an unknown 'scale' (or 'variance') parameter to estimate as well
- The deviance is a generalization of the residual sum of squares.
- The protocols are very similar to linear regression. The inferential logic is virtually identical.

Example: budworms (MASS, Ch. 7)

Classical toxicology study of budworms, by sex.

```
> Budworms <- data.frame(Logdose = rep(0:5, 2),
    Sex = factor(rep(c("M", "F"), each = 6)),
    Dead = c(1, 4, 9, 13, 18, 20, 0, 2, 6, 10,
  12, 16))
> Budworms$Alive <- 20 - Budworms$Dead
> xyplot(Dead/20 ~ I(2^Logdose), Budworms,
     groups = Sex, panel = panel.superpose,
    xlab = "Dose", ylab = "Fraction dead",
    key = list(......), type="b")
```



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Fitting a model and plotting the results

Fitting the model is similar to a linear model

```
> bud.1 <- glm(cbind(Dead, Alive) ~ Sex*Logdose,
   binomial, Budworms, trace=T, eps=1.0e-9)
GLM    linear loop 1: deviance = 5.0137
GLM    linear loop 2: deviance = 4.9937
GLM    linear loop 3: deviance = 4.9937
GLM    linear loop 4: deviance = 4.9937
> summary(bud.1, cor = F)
…
               Value Std. Error  t value
(Intercept) -2.99354    0.55270 -5.41622
        Sex  0.17499    0.77831  0.22483
    Logdose  0.90604    0.16710  5.42207
Sex:Logdose  0.35291    0.26999  1.30713
…
(Residual Deviance: 4.9937 on 8 degrees of freedom
```

```
> bud.0 <- update(bud.1, .~.-Sex:Logdose)
GLM    linear loop 1: deviance = 6.8074
GLM    linear loop 2: deviance = 6.7571
GLM    linear loop 3: deviance = 6.7571
GLM    linear loop 4: deviance = 6.7571
> anova(bud.0, bud.1, test="Chisq")
Analysis of Deviance Table

Response: cbind(Dead, Alive)

          Terms Resid. Df Resid. Dev         Test Df
1 Sex + Logdose         9     6.7571
2 Sex * Logdose         8     4.9937 +Sex:Logdose  1

  Deviance Pr(Chi)
1
2   1.7633 0.18421
```

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Plotting the results

```
attach(Budworms)
plot(2^Logdose, Dead/20, xlab = "Dose",
   ylab = "Fraction dead", type = "n")
text(2^Logdose, Dead/20, c("+","o")[Sex], col = 5,
   cex = 1.25)
newdat <- expand.grid(Logdose = seq(-0.1, 5.1, 0.1),
   Sex = levels(Sex))
newdat$Pr1 <- predict(bud.1, newdat, type = "response")
newdat$Pr0 <- predict(bud.0, newdat, type = "response")
ditch <- newdat$Logdose == 5.1 | newdat$Logdose < 0
newdat[ditch, ] <- NA
attach(newdat)
lines(2^Logdose, Pr1, col=4, lty = 4)
lines(2^Logdose, Pr0, col=3)
```

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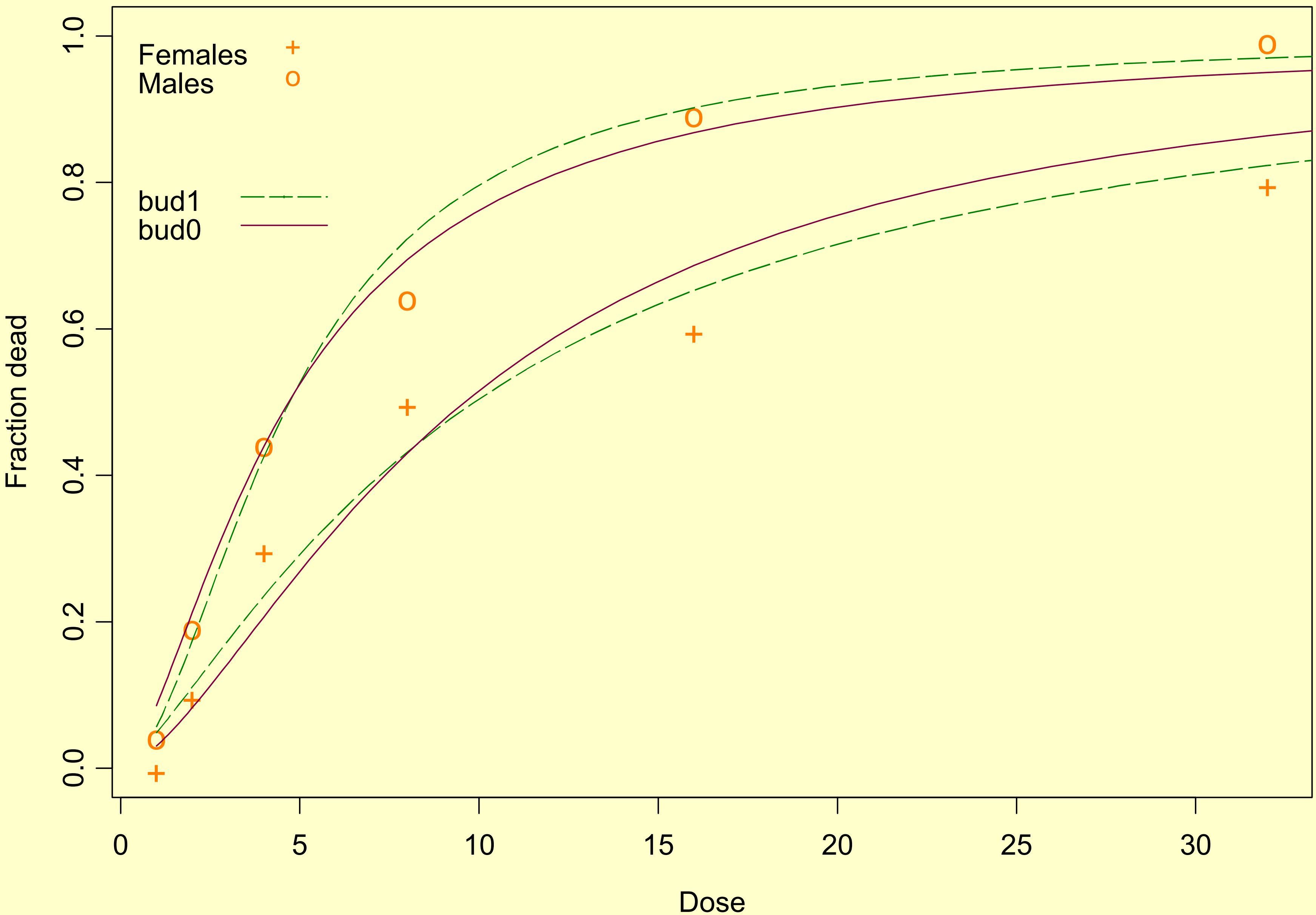
Females +
Males o
bud1
bud0
Fraction dead
0.0
0.2
0.4
0.6
0.8
1.0
0
5
10
15
20
25
30
Dose

Janka data, first re-visit

From transformations it becomes clear that

- A square-root makes the regression straight-line,
- A log is needed to make the variance constant.

One way to accommodate both is to use a GLM with

- Square-root link, and
- Variance proportional to the square of the mean.

This is done using the *quasi family* which allows link and variance functions to be separately specified.

```
family = quasi(link = sqrt, variance = "mu^2")
```


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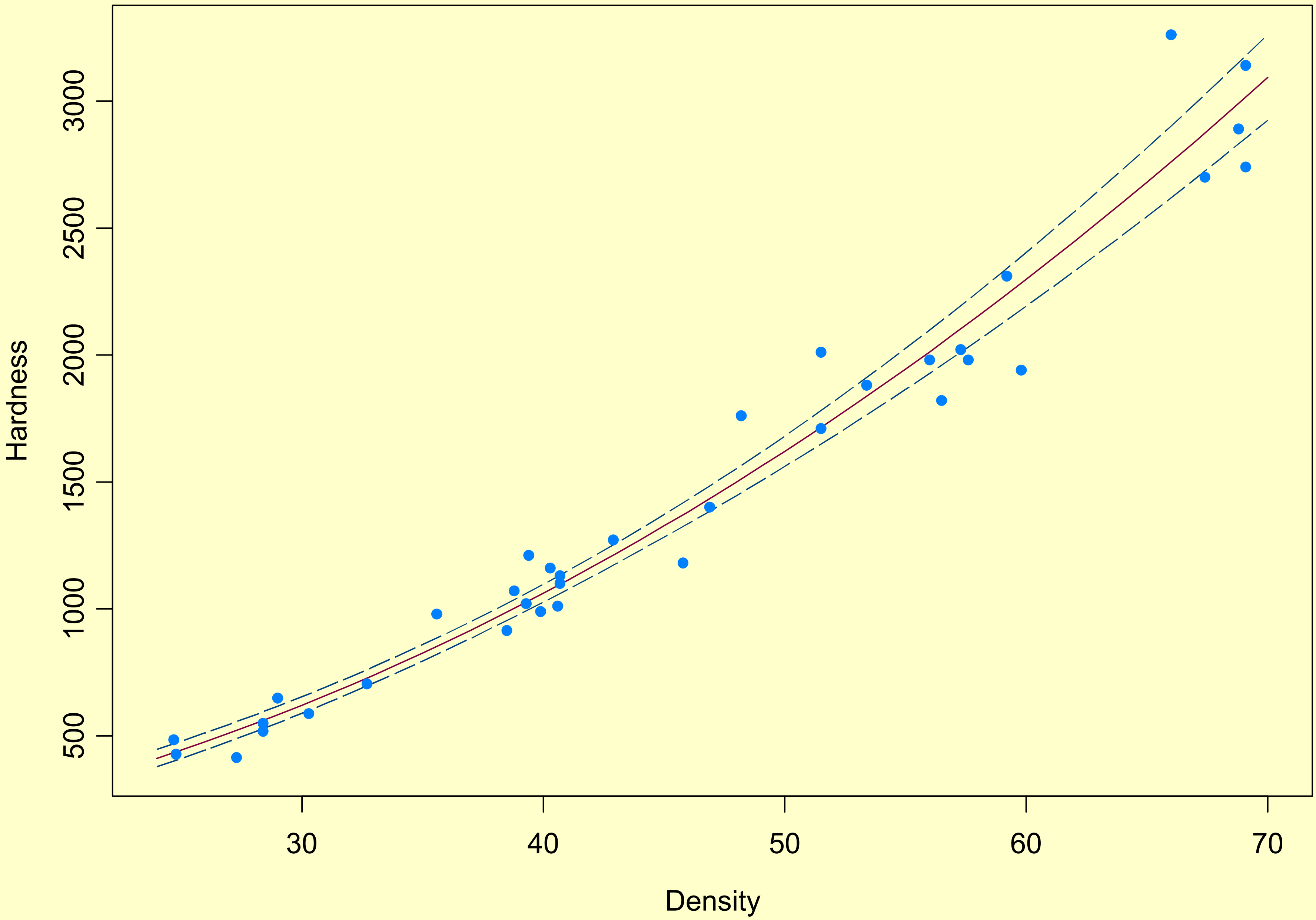
```
> jank.g1 <- glm(Hard ~ Dens, quasi(link = sqrt,
   variance = "mu^2"), janka, trace=T)
GLM    linear loop 1: deviance = 0.3335
GLM    linear loop 2: deviance = 0.3288
GLM    linear loop 3: deviance = 0.3288
> range(janka$Dens)
[1] 24.7 69.1
> newdat <- data.frame(Dens = 24:70)
> p1 <- predict(jank.g1, newdat, type = "response",
                se = T)
> names(p1)
[1] "fit"            "se.fit"         "residual.scale"
[4] "df"
> ul <- p1$fit + 2*p1$se.fit
> ll <- p1$fit - 2*p1$se.fit
> mn <- p1$fit
> matplot(newdat$Dens, cbind(ll, mn, ul),
   xlab = "Density", ylab = "Hardness",
   col = c(2,3,2), lty = c(4,1,4), type = "l")
> points(janka$Dens, janka$Hard, pch=16, col = 6)
```



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Negative Binomial Models

- Useful class of models for count data cases where the variance is much greater than the mean
- A Poisson model to such data will give a deviance much greater than the residual degrees of freedom.
- Has two interpretations
  - As a conditional Poisson model but with an unobserved random effect attached to each observation
  - As a "contagious distribution": the observations are sums of a Poisson number of "clumps" with each clump logarithmically distributed.

The quine data

- Numbers of days absent from school per pupil in a year in a rural NSW town.
- Classified by four factors:

```
> lapply(quine, levels)
$Eth:
[1] "A" "N"
$Sex:
[1] "F" "M"
$Age:
[1] "F0" "F1" "F2" "F3"
$Lrn:
[1] "AL" "SL"
$Days:
NULL
```

First consider a Poisson "full" model"

```
> quine.1 <- glm(Days ~ Eth*Sex*Age*Lrn, poisson, quine,
   trace = T)
…
GLM    linear loop 4: deviance = 1173.9
> quine.1$df
[1] 118
```

Overdispersion. Now a NB model with the same mean structure (and default log link):

```
> quine.n1 <- glm.nb(Days ~ Eth*Sex*Age*Lrn, quine,
   trace=T)
…
Theta( 1 ) = 1.92836 , 2(Ls - Lm) = 167.453
> dropterm(quine.n1, test = "Chisq")
Single term deletions

Model:
Days ~ Eth * Sex * Age * Lrn
                Df    AIC    LRT Pr(Chi)
       <none>      1095.3
Eth:Sex:Age:Lrn  2 1092.7 1.4038 0.49563
```

Manual model building

- Is always risky!
- Is nearly always revealing.

```
> quine.up <- glm.nb(Days ~ Eth*Sex*Age*Lrn, quine)
> quine.m <- glm.nb(Days ~ Eth + Sex + Age + Lrn,
  quine)
> dropterm(quine.m, test="Chisq")
Single term deletions

Model:
Days ~ Eth + Sex + Age + Lrn
       Df    AIC    LRT Pr(Chi)
<none>     1107.2
   Eth  1 1117.7 12.524 0.00040
   Sex  1 1105.4  0.250 0.61728
   Age  3 1112.7 11.524 0.00921
   Lrn  1 1107.7  2.502 0.11372
```

```
> addterm(quine.m, quine.up, test = "Chisq")
Single term additions

Model:
Days ~ Eth + Sex + Age + Lrn
        Df    AIC    LRT Pr(Chi)
 <none>     1107.2
Eth:Sex  1 1108.3  0.881 0.34784
Eth:Age  3 1102.7 10.463 0.01501
Sex:Age  3 1100.4 12.801 0.00509
Eth:Lrn  1 1106.1  3.029 0.08180
Sex:Lrn  1 1109.0  0.115 0.73499
Age:Lrn  2 1110.0  1.161 0.55972

> quine.m <- update(quine.m, .~.+Sex:Age)
> addterm(quine.m, quine.up, test = "Chisq")
```

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```
Single term additions

Model:
Days ~ Eth + Sex + Age + Lrn + Sex:Age
        Df    AIC    LRT Pr(Chi)
 <none>     1100.4
Eth:Sex  1 1101.1  1.216 0.27010
Eth:Age  3 1094.7 11.664 0.00863
Eth:Lrn  1 1099.7  2.686 0.10123
Sex:Lrn  1 1100.9  1.431 0.23167
Age:Lrn  2 1100.3  4.074 0.13043
> quine.m <- update(quine.m, .~.+Eth:Age)
> addterm(quine.m, quine.up, test = "Chisq")
Single term additions

Model:
Days ~ Eth + Sex + Age + Lrn + Sex:Age + Eth:Age
        Df    AIC    LRT Pr(Chi)
 <none>     1094.7
Eth:Sex  1 1095.4 1.2393 0.26560
Eth:Lrn  1 1096.7 0.0004 0.98479
Sex:Lrn  1 1094.7 1.9656 0.16092
Age:Lrn  2 1094.1 4.6230 0.09911
```

```
> dropterm(quine.m, test = "Chisq")
Single term deletions

Model:
Days ~ Eth + Sex + Age + Lrn + Sex:Age + Eth:Age
        Df    AIC    LRT  Pr(Chi)
 <none>    1094.7
    Lrn  1 1097.9  5.166 0.023028
Sex:Age  3 1102.7 14.002 0.002902
Eth:Age  3 1100.4 11.664 0.008628
```

The final model (from this approach) can be written in the form

```
Days ~ Lrn + Age/(Eth + Sex)
```

suggesting that `Eth` and `Sex` have proportional effects nested within `Age`, and `Lrn` has the same proportional effect on all means independent of `Age`, `Sex` and `Eth`.

Generalized Additive Models: Introduction

- Strongly assumes that predictors have been chosen that are unlikely to have interactions between them.
- Weakly assumes a form for the main effect for each term!
- Estimation is done using penalized maximum likelihood where the penalty term uses a measure of roughness of the main effect forms. The tuning constant is chosen automatically by cross-validation.
- Any glm form is possible, but two additional functions, s(x, …) and lo(x,…) may be included, but only additively.
- For many models, spline models can do nearly as well!

Example: The Iowa wheat data revisited

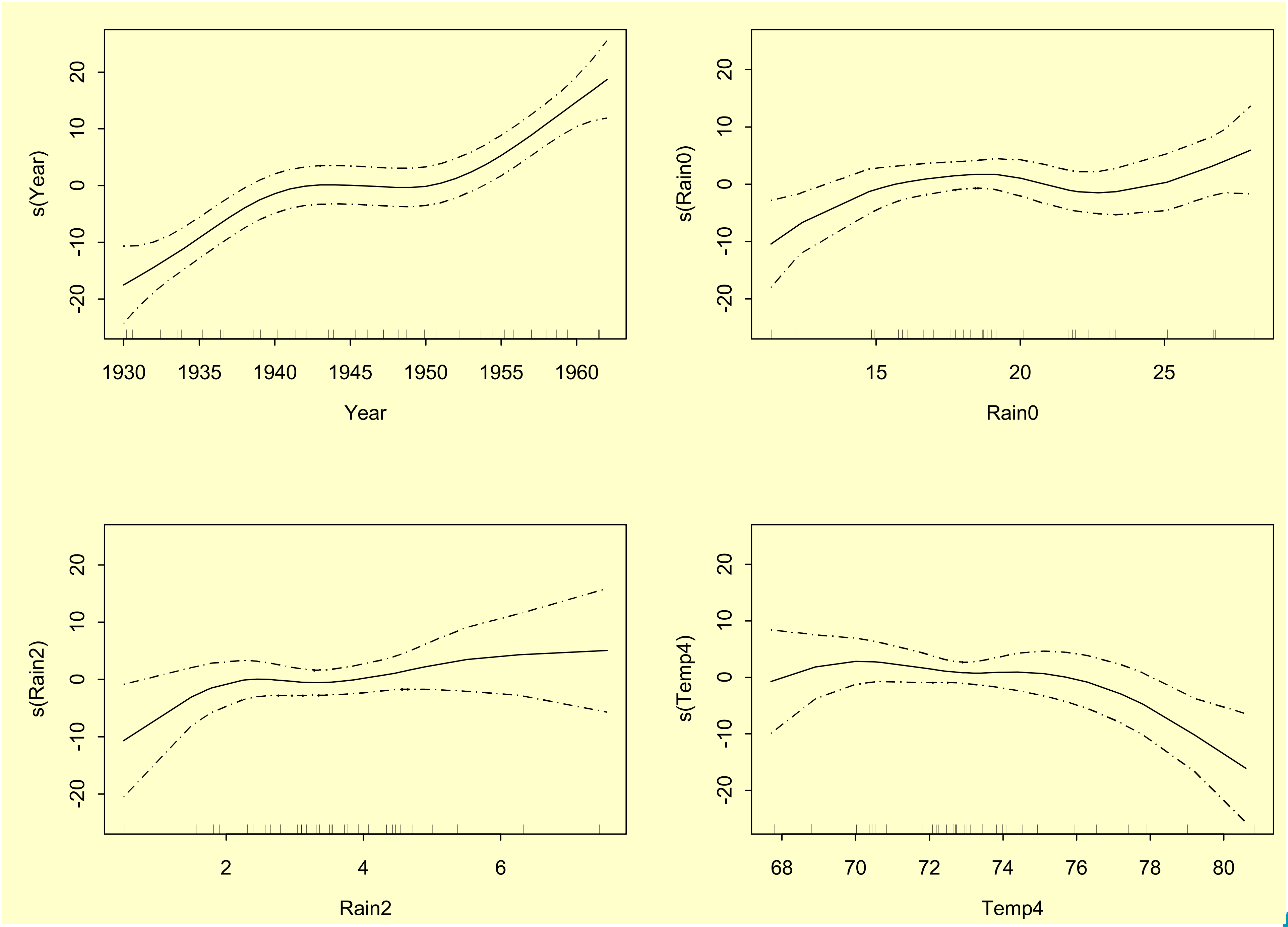
Clear that Year is the dominant predictor.

If any others are useful, `Rain0`, `Rain2` and `Temp4`, at most, could be.

```
> iowa.gm1 <- gam(Yield ~ s(Year) + s(Rain0) +
    s(Rain2) + s(Temp4), data = iowheat)
```

The best way to appreciate the fitted model is to graph the components.

```
> par(mfrow=c(2,2))
> plot(iowa.gm1, se=T, ylim = c(-25, 25))
```



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Comparison with simpler models

```
> Iowa.fakeGAM <- lm(Yield ~ ns(Year, 3) + ns(Rain0, 3)
   + ns(Rain2, 3) + ns(Temp4, 3), iowheat)
> Iowa.fakePol <- lm(Yield ~ poly(Year, 3) +
   poly(Rain0, 3) + poly(Rain2, 3) + poly(Temp4, 3),
   iowheat)

> par(oma = c(0,0,4,0))

> plot.gam(Iowa.fakeGAM, se=T, ylim = c(-25, 25))
> mtext("Additive components of a simple spline model",
   outer = T, cex = 2)

> plot.gam(Iowa.fakePol, se=T, ylim = c(-25, 25))
> mtext("Additive components of a cubic polynomial
   model", outer = T, cex = 2)
```


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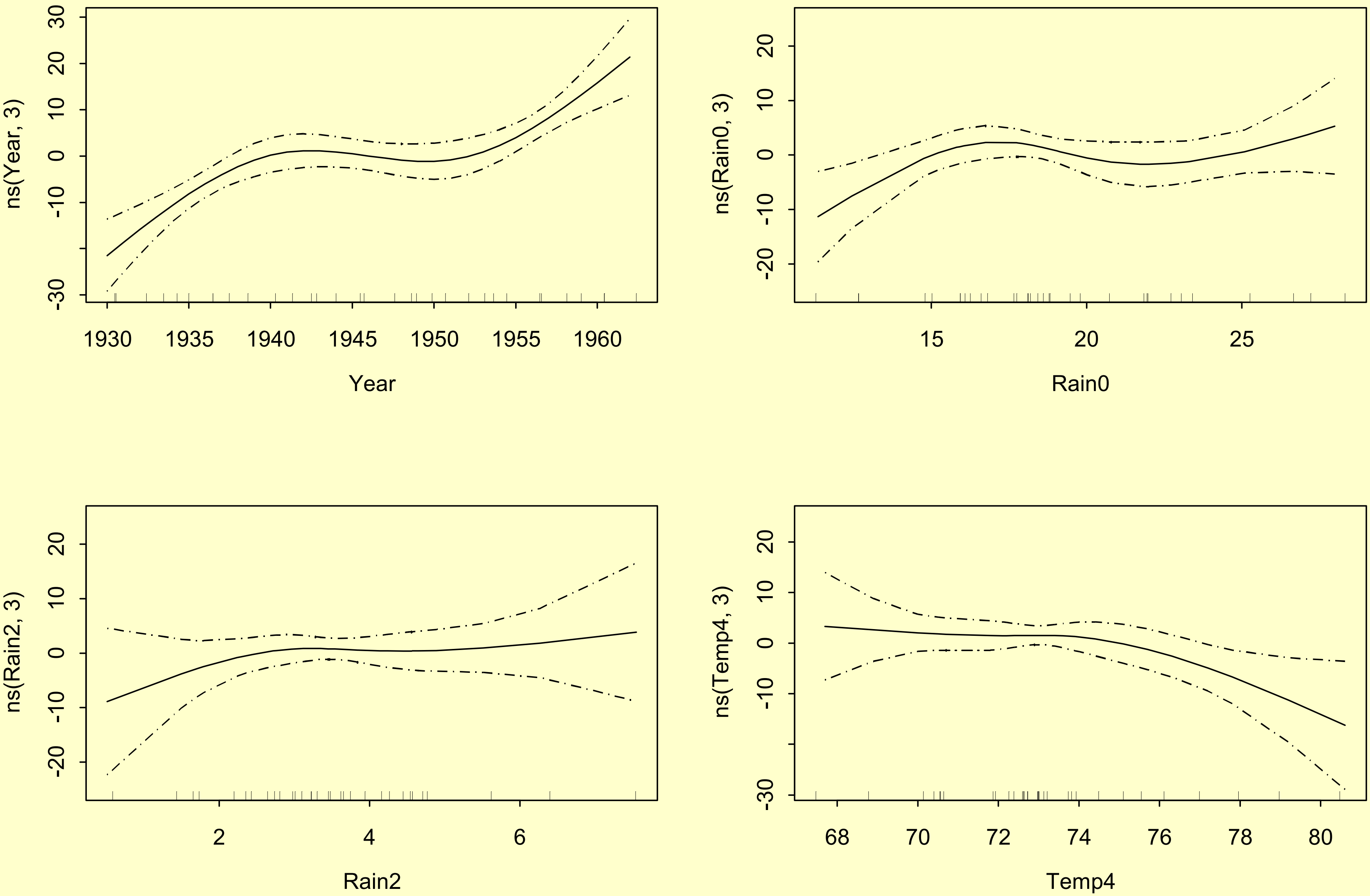
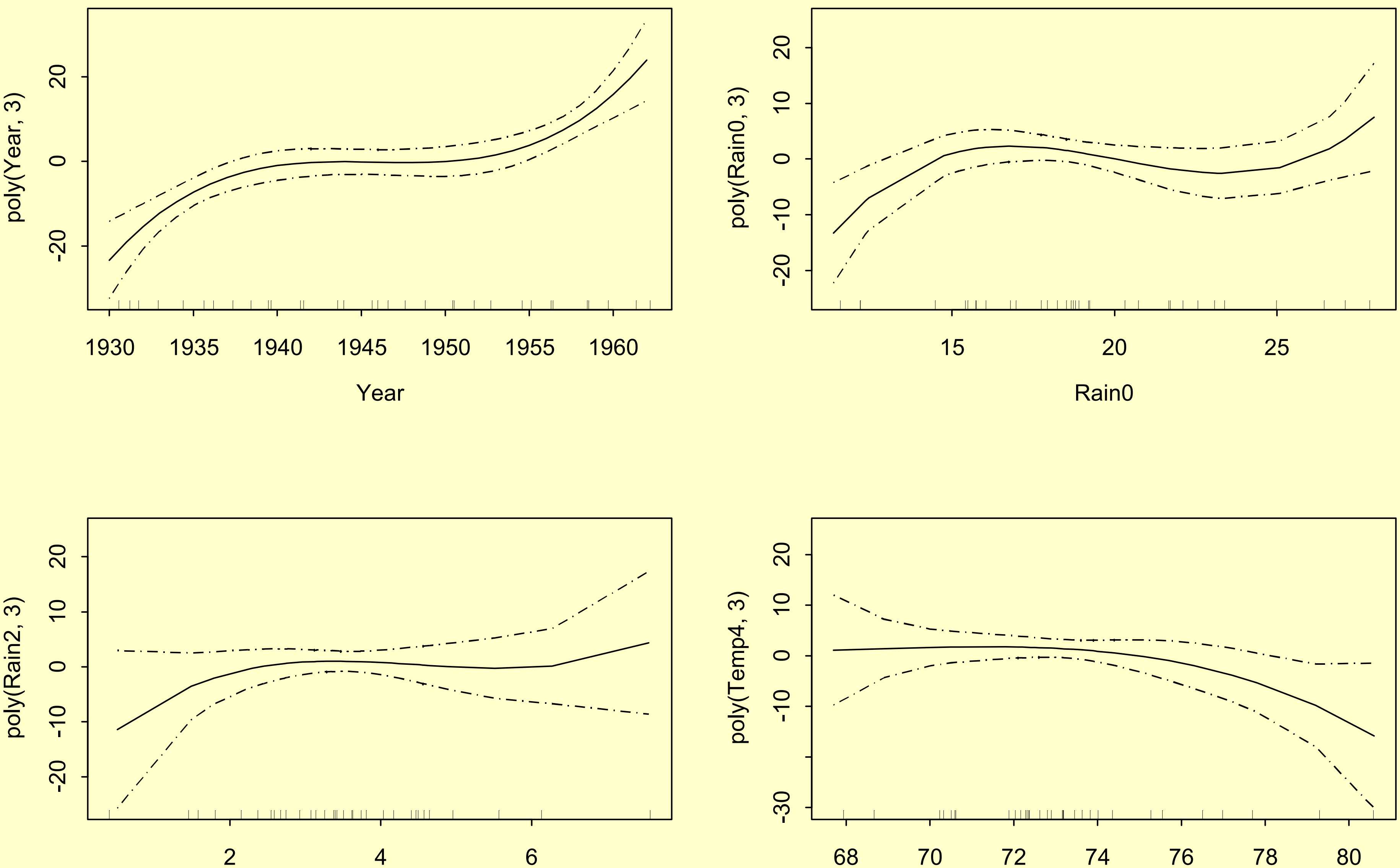
Additive components of a simple spline model



Additive components of a cubic polynomial model



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GLMs with Random Effects

- This is still a controversial area (Nelder, Goldstein, Diggle, …)
- Practice is not waiting for theory!
- Breslow & Clayton two procedures: "penalized quasi-likelihood" and "marginal quasi-likelihood (PQL & MQL)
- MQL is rather like estimating equations; PQL is much closer to the spirit of random effects.
- glmmPQL is part of the MASS library and implements PQL using the B&C algorithm. Should be used carefully, though for most realistic data sets the method is probably safe enough.

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A test: the quine data with Poisson PQL

- The negative binomial model has an interpretation as a poisson model with a single random effect for each observation.
- If the random effect has a 'log of gamma' distribution the exact likelihood can be computed and maximized (`glm.nb`).
- If the random effect has a normal distribution the integration is not feasable and approximate methods of estimation are needed.
- The two models, in principle, should be very similar. Are they in practice?

First, re-fit the preferred NB model:

```
> quine.nb <- glm.nb(Days ~ Lrn +
                  Age/(Eth + Sex), quine)
```

Now make a local copy of quine, add the additional component and fit the (large) random effects model:

```
> quine <- quine
> quine$Child <- factor(1:nrow(quine))
> library(MASS, first = T)
> quine.re <- glmmPQL(Days ~ Lrn +
  Age/(Eth + Sex), family = poisson(link = log),
  data = quine, random = ~1 | Child, maxit = 20)
iteration 1
iteration 2
...
iteration 10
```

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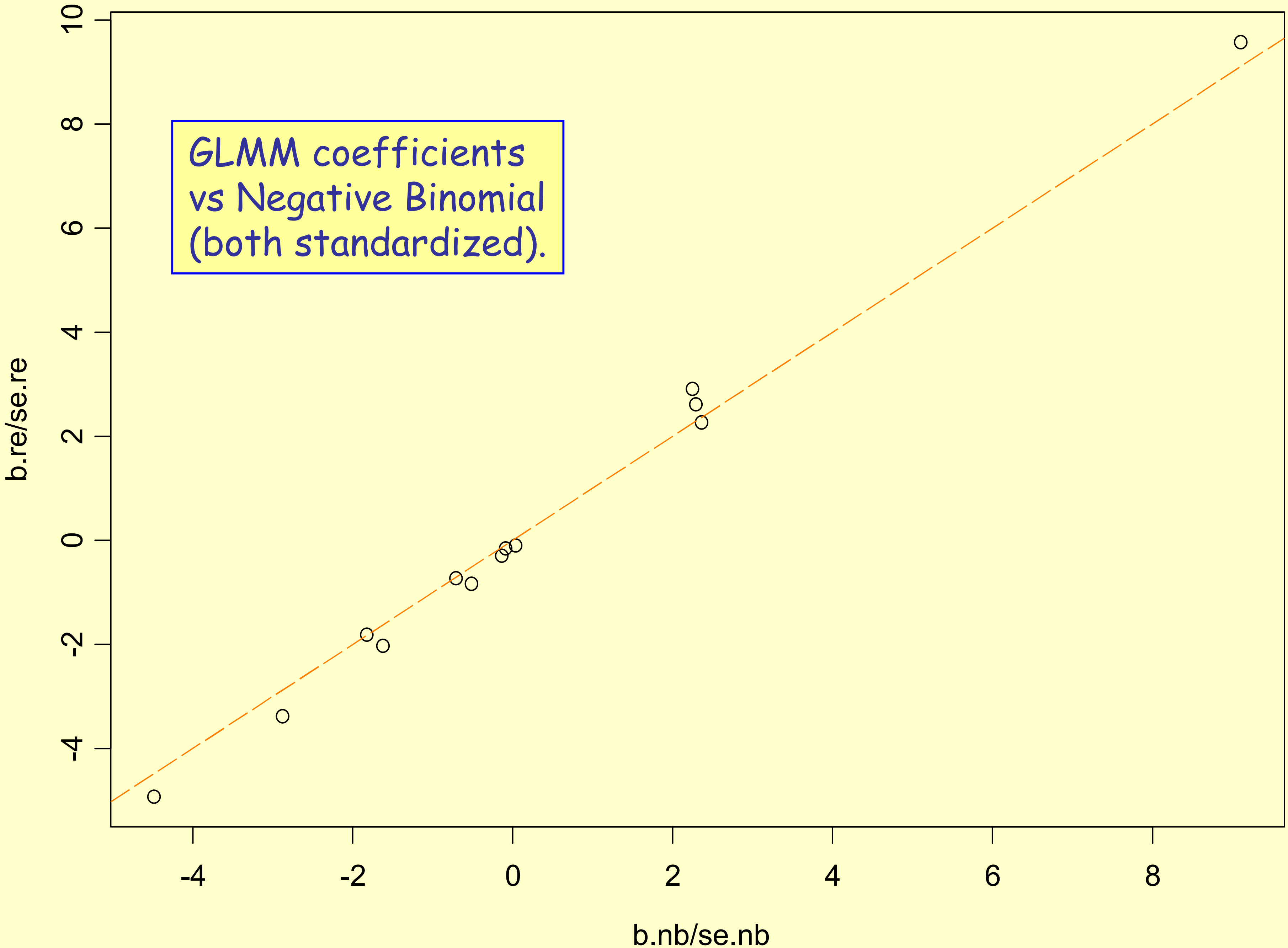
How similar are the coefficients (and SE)?

```
> b.nb <- coef(quine.nb)
> b.re <- fixed.effects(quine.re)
> rbind(NB = b.nb, RE = b.re)
   (Intercept)      Lrn    AgeF1     AgeF2    AgeF3
NB      2.8651 0.43464 -0.26946 -0.035837 -0.20542
RE      2.6889 0.36301 -0.24835 -0.058735 -0.30111

    AgeF0Eth AgeF1Eth AgeF2Eth  AgeF3Eth AgeF0Sex AgeF1Sex
NB  0.012582 -0.74511  -1.2082 -0.040114 -0.54904 -0.52050
RE -0.030215 -0.76261  -1.1759 -0.079303 -0.61111 -0.44163

   AgeF2Sex AgeF3Sex
NB  0.66164  0.66438
RE  0.66571  0.77235
```

```
> se.re <- sqrt(diag(quine.re$varFix))
> se.nb <- sqrt(diag(vcov(quine.nb)))
> rbind(se.re, se.nb)
         [,1]    [,2]    [,3]    [,4]    [,5]    [,6]
se.re 0.28100 0.16063 0.33832 0.36867 0.35762 0.29025
se.nb 0.31464 0.18377 0.37982 0.41264 0.40101 0.32811

         [,7]    [,8]    [,9]   [,10]   [,11]   [,12]
se.re 0.22531 0.23852 0.26244 0.30130 0.24281 0.25532
se.nb 0.25926 0.26941 0.29324 0.33882 0.28577 0.28857

        [,13]
se.re 0.26538
se.nb 0.29553
> plot(b.nb/se.nb, b.re/se.re)
> abline(0, 1, col = 3, lty = 4)
```


GLMM coefficients
vs Negative Binomial
(both standardized).
b.re/se.re
b.nb/se.nb
-4
-2
0
2
4
6
8
10

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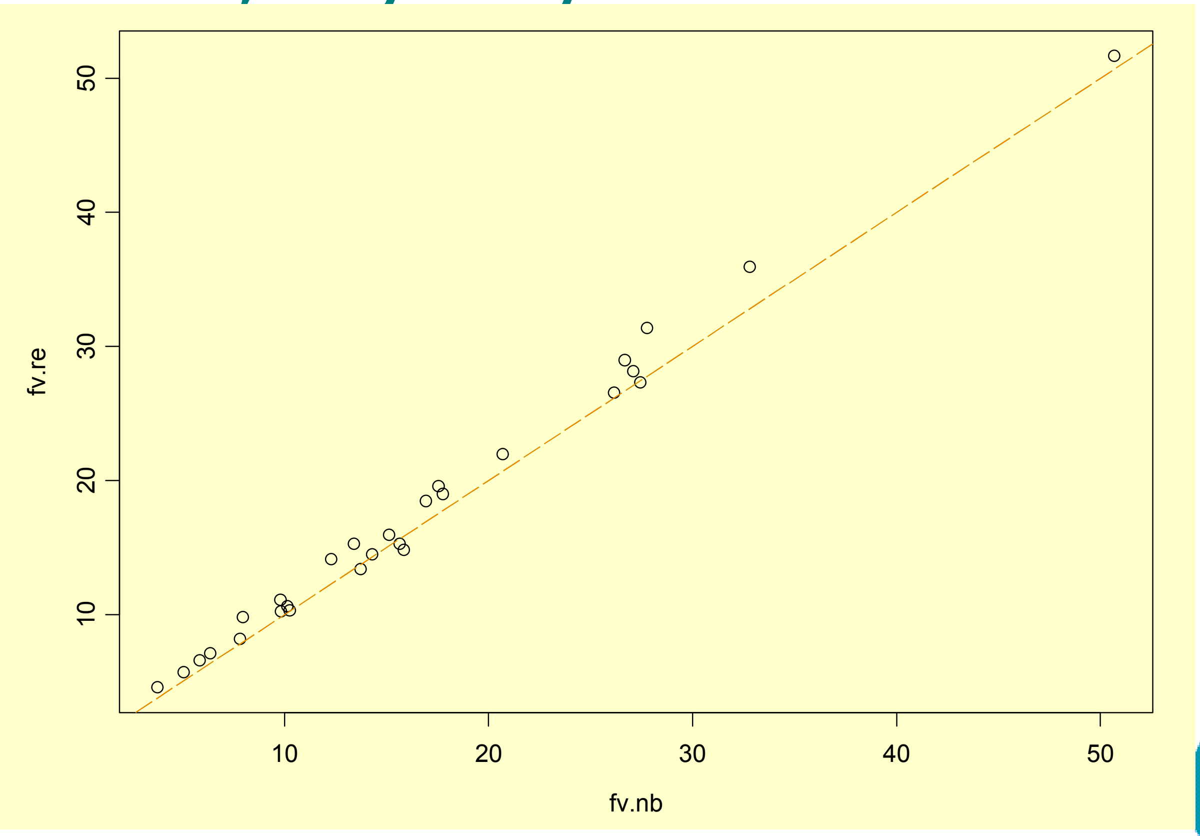
Comparing predictions

- The negative binomial fitted values should be comparable with the "level 0" predictions from the GLMM, i.e. fixed effects only.
- The predict generic function predicts on the link scale. For the GLMM we need a correction to go from the log scale to the direct scale (cf. lognormal distribution).
- An approximate correction (on the log scale) is $\sigma^2/2$ where σ^2 is the variance of the random effects (or BLUPs).

```
> fv.nb <- fitted(quine.nb)
> fv.re <- exp(predict(quine.re, level = 0) +
  var(random.effects(quine.re))/2)
> plot(fv.re, fv.nb)
> plot(fv.nb, fv.re)
> abline(0, 1, col = 5, lty = 4)
```

GLMM vs NB predictions on the original scale.



Non-linear regression

- Generalization of linear regression.
- Normality and equal variance retained, linearity of parameters relaxed.
- Generally comes from a fairly secure theory; not often appropriate for empirical work
- Estimation is still by least squares (= maximum likelihood), but the sum of squares surface is not necessarily quadratic.
- Theory is approximate and relies on SSQ surface being *nearly* quadratic in a region around the minimum.

The Stormer Viscometer Data

SUMMARY:

The stormer viscometer measures the viscosity of a fluid by measuring the time taken for an inner cylinder in the mechanism to perform a fixed number of revolutions in response to an actuating weight. The viscometer is calibrated by measuring the time taken with varying weights while the mechanism is suspended in fluids of accurately known viscosity. The data comes from such a calibration, and theoretical considerations suggest a non-linear relationship between time, weight and viscosity, of the form

$$T = \frac{\beta_1 V}{W - \beta_2} + \varepsilon$$

where β_1 and β_2 are unknown parameters to be estimated, and E is error.

DATA DESCRIPTION:

The data frame contains the following components:

ARGUMENTS:

`Viscosity`	Viscosity of fluid
`Wt`	Actuating weight
`Time`	Time taken

SOURCE:

E. J. Williams (1959) *Regression Analysis.* Wiley.

A simple example

- Stormer viscometer data (data frame `stormer` in MASS).

```
> names(stormer)
[1] "Viscosity" "Wt"        "Time"
```

- Model:

$$T = \beta V/(W - \theta) + error$$

- Ignoring *error* and re-arranging gives:

$$WT \simeq \beta V + \theta T$$

- Fit this relationship with ordinary least squares to get initial values for β and θ.

Fitting the model

Is very easy for this example…

```
> b <- coef(lm(Wt*Time ~ Viscosity + Time - 1,
                                         stormer))
> names(b) <- c("beta", "theta")
> b
   beta  theta
 28.876 2.8437
> storm.1 <-
    nls(Time ~ beta*Viscosity/(Wt - theta),
                           stormer, start=b, trace=T)
885.365 : 28.8755 2.84373
825.110 : 29.3935 2.23328
825.051 : 29.4013 2.21823
```

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Looking at the results

```
> summary(storm.1)
Formula: Time ~ (beta * Viscosity)/(Wt - theta)

Parameters:
        Value Std. Error t value
 beta 29.4013    0.91553 32.1138
theta  2.2182    0.66552  3.3331

Residual standard error: 6.26803 on 21 degrees of
   freedom

Correlation of Parameter Estimates:
       beta
theta -0.92
```


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Self-starting models

Allows the starting procedure to be encoded into the model function.
(Somewhat arcane but very powerful)

```
> library(nls)                                         # R only
> library(MASS)
> data(stormer)                                        # R only
> storm.init <- function(mCall, data, LHS) {
      v <- eval(mCall[["V"]], data)
      w <- eval(mCall[["W"]], data)
      t <- eval(LHS, data)
      b <- lsfit(cbind(v, t), t * w, int = F)$coef
      names(b) <- mCall[c("b", "t")]
      b
    }
> NLSstormer <- selfStart( ~ b*V/(W-t),
       storm.init, c("b","t"))
> args(NLSstormer)
function(V, W, b, t)
NULL …
```

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```
> tst <- nls(Time ~ NLSstormer(Viscosity, Wt, beta,
                          theta), stormer, trace = T)
885.365 : 28.8755 2.84373
825.110 : 29.3935 2.23328
825.051 : 29.4013 2.21823
```

Bootstrapping is NBD:

```
> tst$call$trace <- NULL
> B <- matrix(NA, 500, 2)
> r <- scale(resid(tst), scale = F)      # mean correct
> f <- fitted(tst)
> for(i in 1:500) {
       v <- f + sample(r, rep = T)
       B[i, ] <- try(coef(update(tst, v ~ .))) # guard!
  }
> cbind(Coef = colMeans(B), SD = colStdevs(B))
        Coef       SD
[1,] 29.4215 0.64390
[2,]  2.2204 0.46051
```

NLS example: the muscle data

- Old data from an experiment on muscle contraction in experimental animals.
- *Variables*:
  - `Strip`: identifier of muscle (animal)
  - `Conc`: CaCl concentrations used to soak the section
  - `Length`: resulting length of muscle section for each concentration
- *Model*: $$L = \alpha + \beta \exp(-C/\theta) + error$$

  where α and β may vary with the animal but θ is constant.
- Note that α and β are (very many) linear parameters. We use this strongly

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First model: fixed parameters

- Since there are 21 animals with separate alpha's and beta's for each the number of parameters is 21+21+1=43, from 61 observations!
- Use the *plinear* algorithm since all parameters are linear bar one.

```
> X <- model.matrix(~ Strip - 1, muscle)
> musc.1 <- nls(Length ~ cbind(X, X*exp(-Conc/th)),
    muscle, start = list(th = 1), algorithm = "plinear",
    trace = T)
....
> b <- coef(musc.1)
> b
      th   .lin1  .lin2  .lin3  .lin4 .lin5 .lin6  .lin7
 0.79689 23.454 28.302 30.801 25.921  23.2 20.12 33.595
  ......
  .lin39 .lin40  .lin41  .lin42
 -15.897 -28.97 -36.918 -26.508
```

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Conventional fitting algorithm

- Parameters in non-linear regression may be indexed:

```
> th <- b[1]
> a <- b[2:22]
> b <- b[23:43]
> musc.2 <- nls(Length ~ a[Strip] +
       b[Strip)*exp(-Conc/th),
       muscle, start = list(a = a, b = b, th = th),
       trace = T)
  ......
```

- Converges in one step, now.
- Note that with indexed parameters, the starting values must be given in a list (with names).

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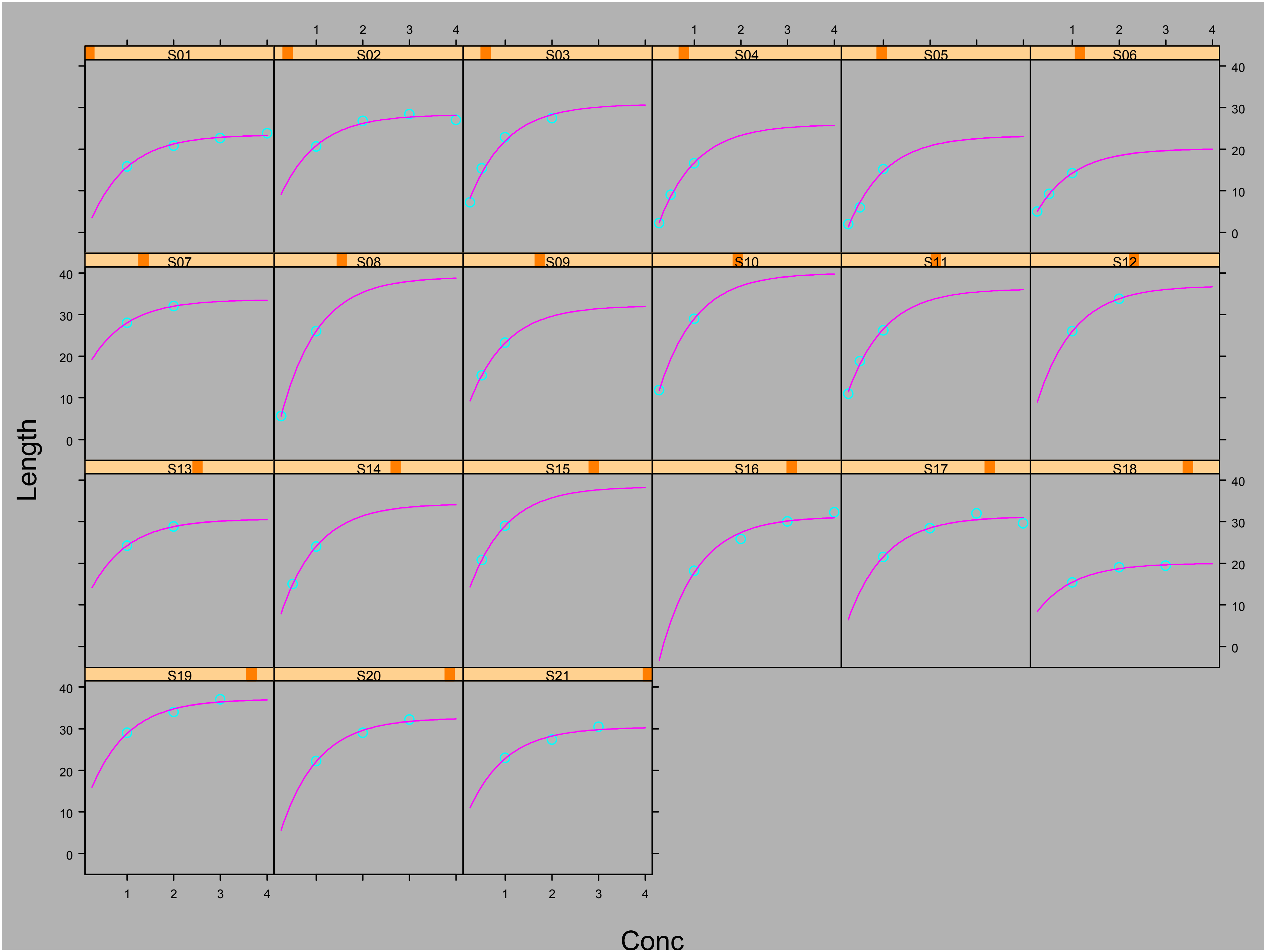
Plotting the result

```
> range(muscle$Conc)
[1] 0.25 4.00
> newdat <- expand.grid(
             Strip = levels(muscle$Strip),
             Conc = seq(0.25, 4, 0.05))
> dim(newdat)
[1] 1596    2
> names(newdat)
[1] "Strip" "Conc"
> newdat$Length <- predict(musc.2, newdat)
```

The actual plot

Trellis comes to the rescue:

```
> xyplot(Length ~ Conc | Strip, muscle, subscripts = T,
    panel = function(x, y, subscripts, ...) {
        panel.xyplot(x, y, ...)
        ws <- as(muscle$Strip[subscripts[1]], "character")
        wf <- which(newdat$Strip == ws)
        xx <- newdat$Conc[wf]
        yy <- newdat$Length[wf]
        lines(xx, yy, col = 3)
    }, ylim = range(newdat$Length, muscle$Length),
    as.table = T)
```



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A Random Effects version

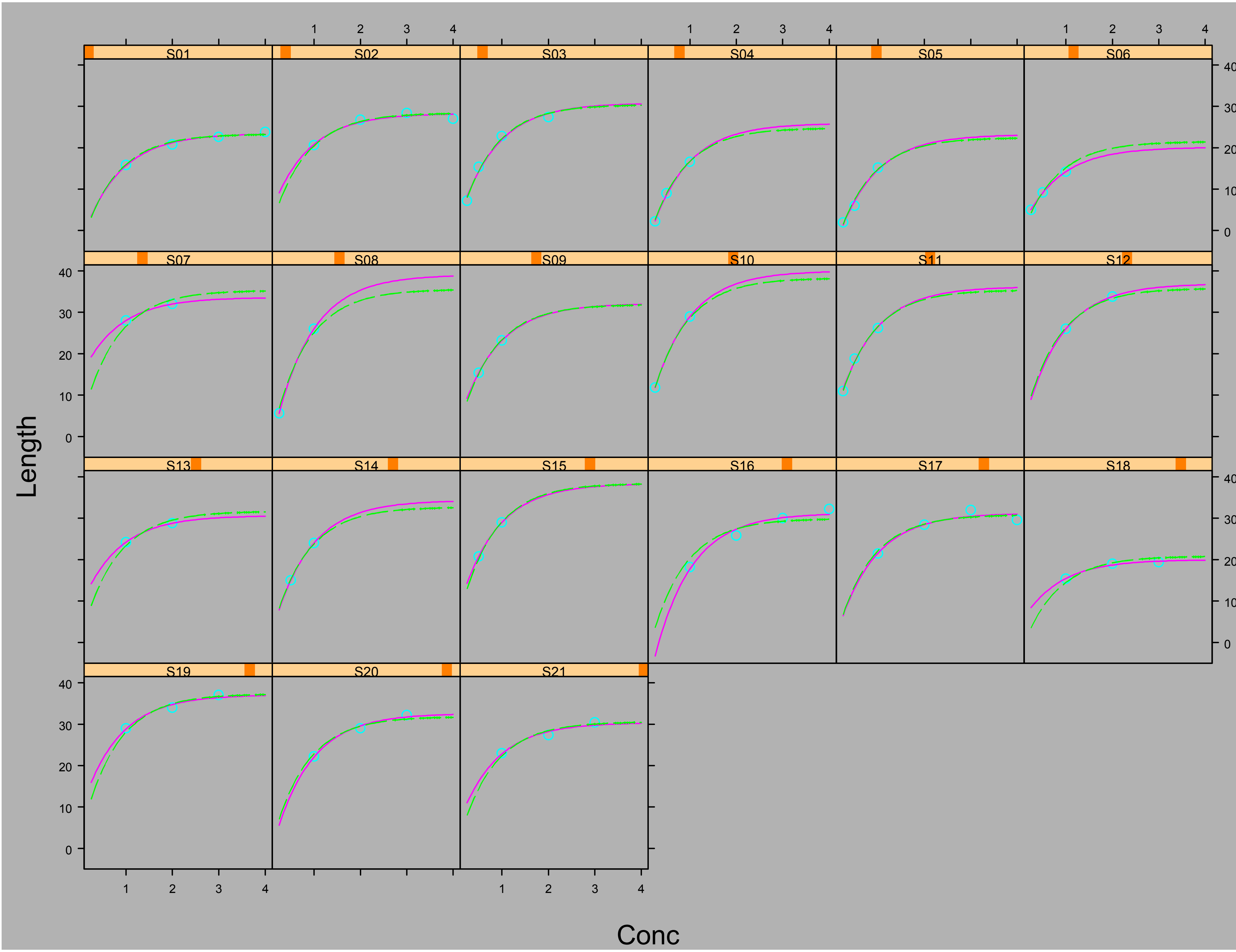
- Random effects models allow the parametric dimension to be more easily controlled.
- We assume α and β are now random over animals

```
> musc.re <- nlme(Length ~ a + b*exp(-Conc/th),
      fixed = a+b+th~1, random = a+b~1|Strip,
      data = muscle, start =
            c(a=mean(a), b=mean(b), th=th))
```

- The vectors `a`, `b` and `th` come from the previous fit; no need to supply initial values for the random effects, (though you may).

A composite plot

```
> newdat$L2 <- predict(musc.re, newdat)
> xyplot(Length ~ Conc | Strip, muscle, subscripts = T,
   panel =
     function(x, y, subscripts, ...) {
         panel.xyplot(x, y, ...)
  ws <- as(muscle$Strip[subscripts[1]], "character")
         wf <- which(newdat$Strip == ws)
         xx <- newdat$Conc[wf]
         yy <- newdat$Length[wf]
         lines(xx, yy, col = 3)
         yy <- newdat$L2[wf]
         lines(xx, yy, lty=4, col=4)
     }, ylim = range(newdat$Length, muscle$Length),
   as.table = T)
```



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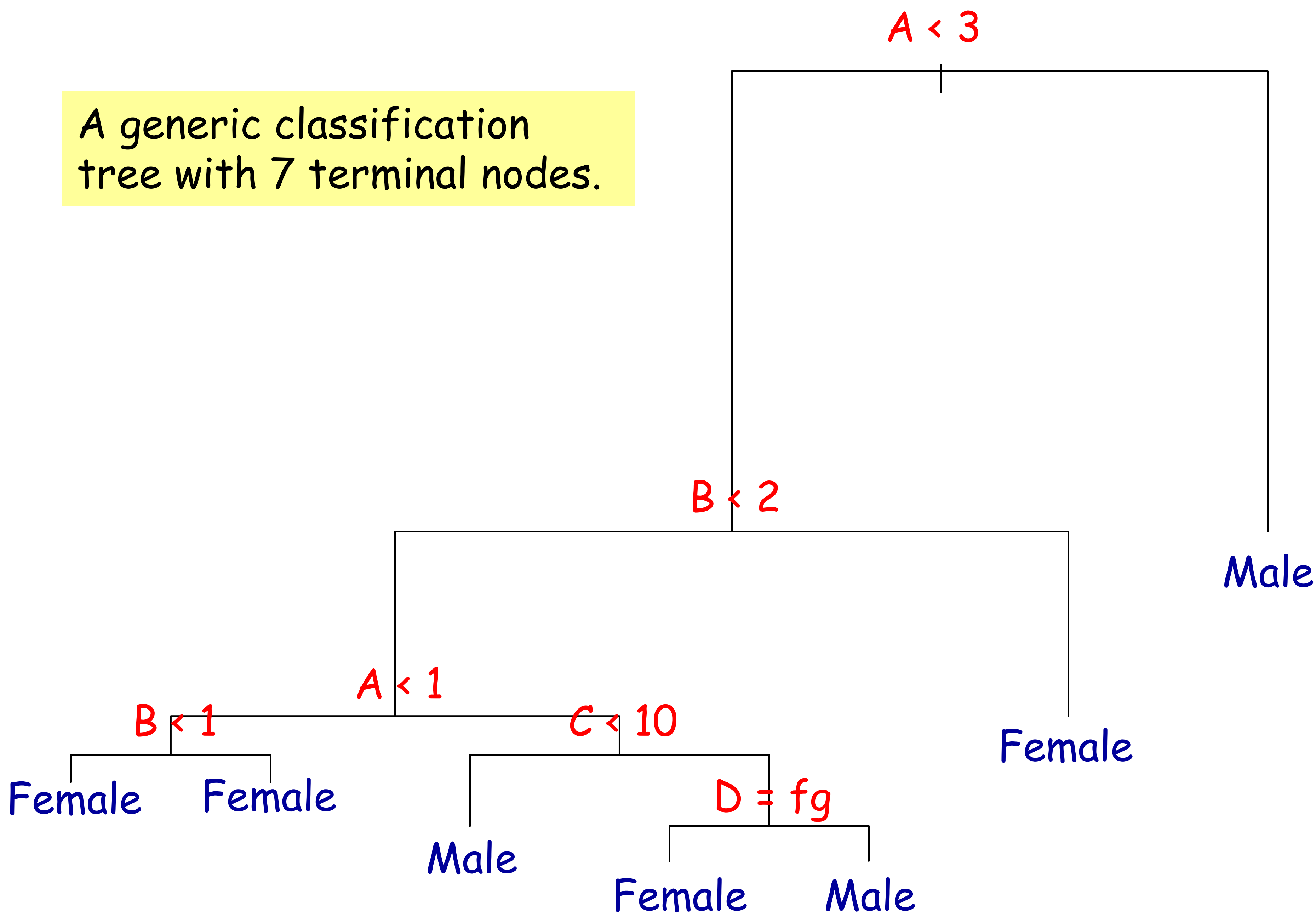
Tree based methods - an introduction

V&R, Ch. 9 (formerly 10).

- A *decision tree* is a sequence of binary rules leading to one of a number of *terminal nodes*, each associated with some decision.
- A *classification tree* is a decision tree that attempts to reproduce a given classification as economically as possible.
- A variable is selected and the population is divided into two at a selected breakpoint of that variable.
- Each half is then independently subdivided further on the same principle, thus recursively forming a binary tree structure.
- Each node is associated with a *probability forecast* for membership in each class (hopefully as specific as possible).

A generic classification tree with 7 terminal nodes.



Trees, more preliminaries

- The faithfulness of any classification tree is measured by a *deviance* measure, $D(T)$, which takes its miminum value at zero if every member of the training sample is uniquely and correctly classified.
- The *size* of a tree is the number of terminal nodes.
- A *cost-complexity measure* of a tree is the deviance penalized by a multiple of the size:

$$D(T) = D(T) + \alpha \,\mathrm{size}(T)$$

where α is a tuning constant. This is eventually minimized.

- Low values of α for this measure imply that accuracy of prediction (in the training sample) is more important than simplicity.
- High values of α rate simplicity relatively more highly than predictive accuracy.

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Regression trees

- Suppose Y has a distribution with mean depending on several determining variables, not necessarily continuous.
- A *regression tree* is a decision tree that partitions the determining variable space into non-overlapping *prediction regions*.
- Within each prediction region the response variable Y is predictied by a constant.
- The deviance in this case is exactly the same as for regression: the residual sum of squares.
  - With enough regions (nodes) the training sample can clearly be reproduced exactly, but predictions will be inaccurate.
  - With too few nodes predictions may be seriously biased.
- *How many nodes should we use?* This is the key question for all of tree modelling (equivalent to setting the tuning constant).

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Some S tree model facilities

```
ftr <- tree(formula, data = dataFrame, ...)
rtr <- rpart(formula, data = dataFrame, ...)
```

implements an algorithm to produce a binary tree (regression or classification) and returns a *tree object*.

The *formula* is of the simple form

`R ~ X1 +X2 +  …`

where `R` is the target variable and `X1, X2, ...` are the determining variables.

if `R` is a factor the result is a classification tree,

if `R` is numeric the result is a regression tree.

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`tree` or `rpart`?

- In S-PLUS there is a native tree library that V&R have some reservations about. It is useful, though.
- **`rpart`** is a library written by Beth Atkinson and Terry Therneau of the Mayo Clinic, Rochester, NY. It is much closer to the spirit of the original CART algorithm of Breiman, *et al*. It is now supplied with both S-PLUS and R.
- In R, there is a **`tree`** library that is an S-PLUS look-alike, but we think better in some respects.
- **`rpart`** is the more flexible and allows various splitting criteria and different model bases (survival trees, for example).
- **`rpart`** is probably the better package, but **`tree`** is acceptable and some things such as cross-validation are easier with tree.
- In this discussion we (nevertheless) largely use **`tree`**!

Some other arguments to `tree`

There are a number of other optional important arguments, for example:

```
na.action = na.omit
```

indicates that cases with missing observations on some requried variable are to be omitted.

By default the algorithm terminates the splitting when the group is either homogeneous or of size 5 or less. Occasionally it is useful to remove or tighten this restriction, and so

```
minsize = k
```

specifics that the groups may be as small as **`k`**.

Displaying and interrogating a tree

```
> plot(ftr)
> text(ftr)
```

will give a graphical representation of the tree, as well as text to indicate how the tree has been constructed.

The assignment

```
> nodes <- identify(ftr)
```

allows interactive identification of the cases in each node.

Clicking on any node produces a list of row labels in the working window.

Clicking on the right button terminates the interactive action.

The result is an S list giving the contents (as character string vector components) of the nodes selected.

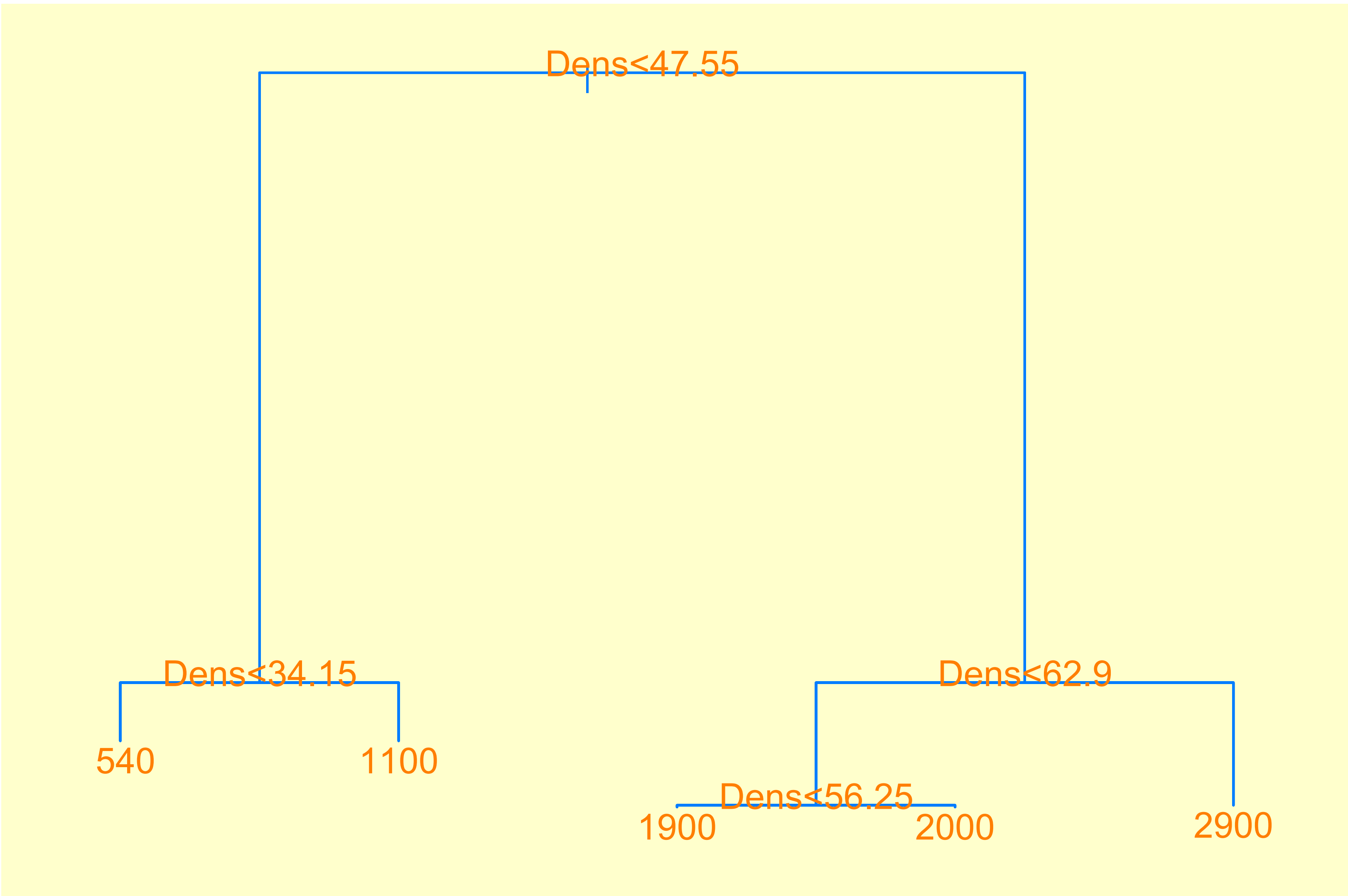
An simplistic example: The Janka data

Consider predicting trees by, well, trees!

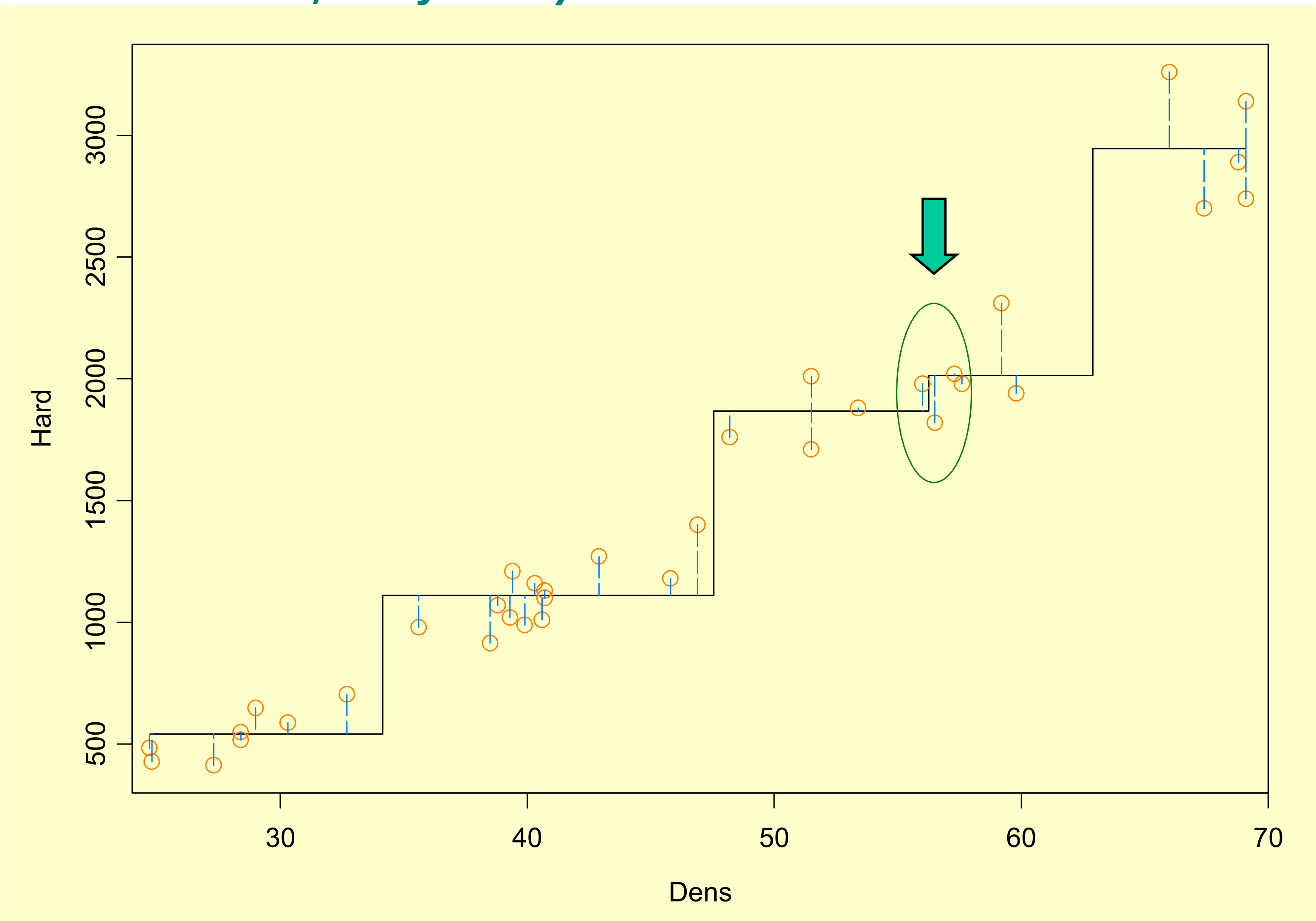
```
> jank.t1 <- tree(Hard ~ Dens, janka)
> jank.t1
node), split, n, deviance, yval
      * denotes terminal node
 1) root 36 22000000 1500
   2) Dens<47.55 21  1900000 890
     4) Dens<34.15 8    73000  540 *
     5) Dens>34.15 13   220000 1100 *
   3) Dens>47.55 15  3900000 2300
     6) Dens<62.9 10   250000 1900
      12) Dens<56.25 5    69000 1900 *
      13) Dens>56.25 5   130000 2000 *
     7) Dens>62.9 5   240000 2900 *
```

The tree has 5 terminal nodes. We can take two views of the model that complement each other.

```
> plot(jank.t1, lwd = 2, col = 6)
> text(jank.t1, cex = 1.25, col = 5)
```



```
> partition.tree(jank.t1, xlim = c(24, 70))
> attach(janka)
> points(Dens, Hard, col = 5, cex = 1.25)
> segments(Dens, Hard, Dens, predict(jank.t1),
      col = 6, lty = 4)
```



A classification tree: Bagging

- Survey data (data frame survey from the MASS library).

```
> ?survey
> names(survey)
 [1] "Sex"     "Wr.Hnd" "NW.Hnd" "W.Hnd"  "Fold"   "Pulse"
 [7] "Clap"    "Exer"   "Smoke"  "Height" "M.I"    "Age"
```

- We consider predicting Sex from the other variables.
- Remove cases with missing values
- Split data set into "Training" and "Test" sets
- Build model in training set, test in test.
- Look at simple "bagging" to improve stability and predictions

Preliminary manipulations

We start with a bit of data cleaning.

```
> dim(survey)
[1] 237  12
> count.nas <- function(x) sum(is.na(x))
> sapply(survey, count.nas)
 Sex Wr.Hnd NW.Hnd W.Hnd Fold Pulse Clap Exer Smoke Height
   1      1      1     1    0    45    1    0     1     28
 M.I Age
  28   0
> Srvy <- na.omit(survey)
> dim(Srvy)
[1] 168  12
```

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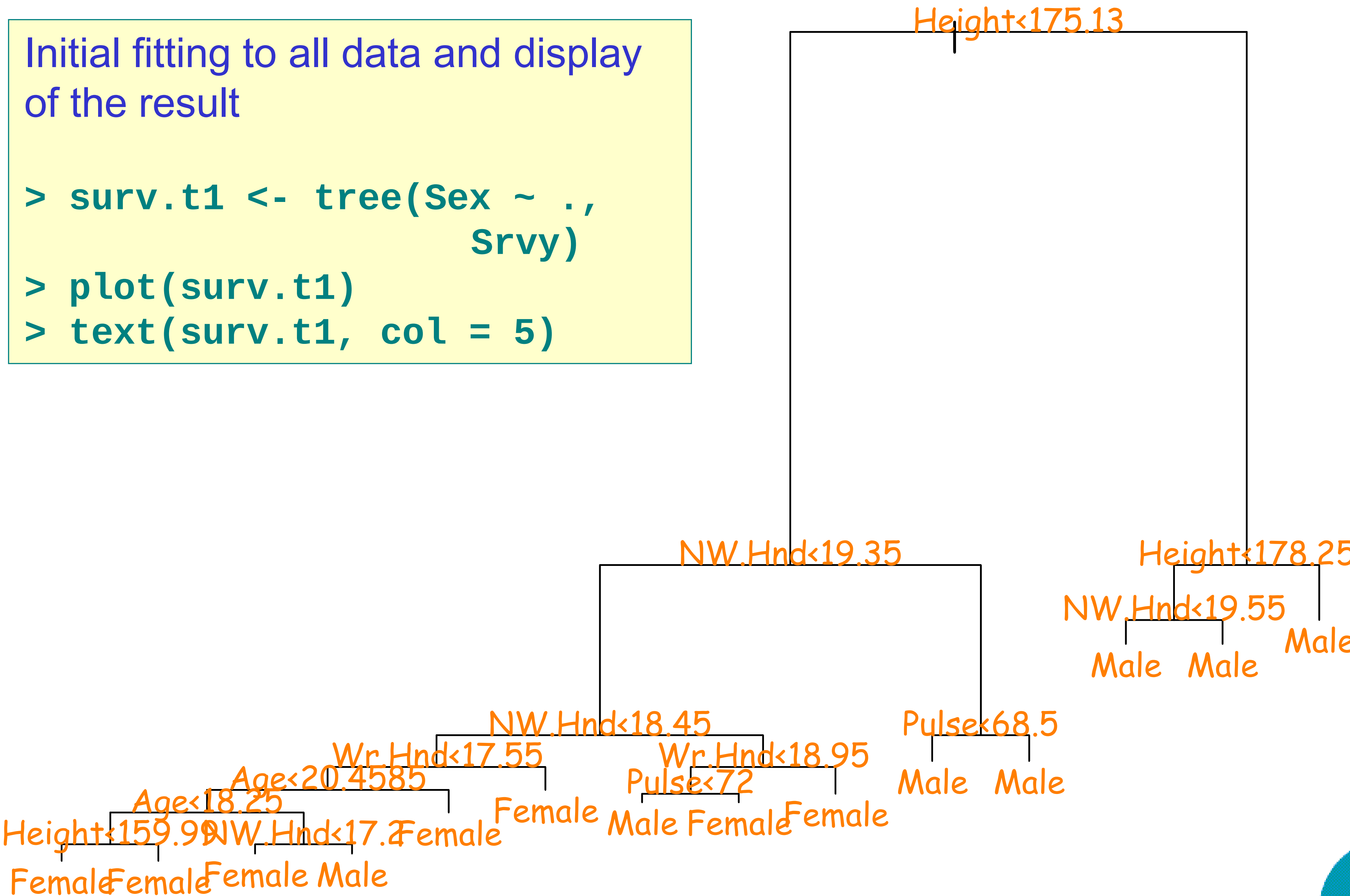
Initial fitting to all data and display of the result

```
> surv.t1 <- tree(Sex ~ .,
                    Srvy)
> plot(surv.t1)
> text(surv.t1, col = 5)
```



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Cross-validation

A technique for using internal evidence to guage the size of tree warranted by the data.

Random sections are omitted and the remainder used to construct a tree. The ommitted section is then predicted from the remainder and various criteria (deviance, error rate) used to assess the efficacy.

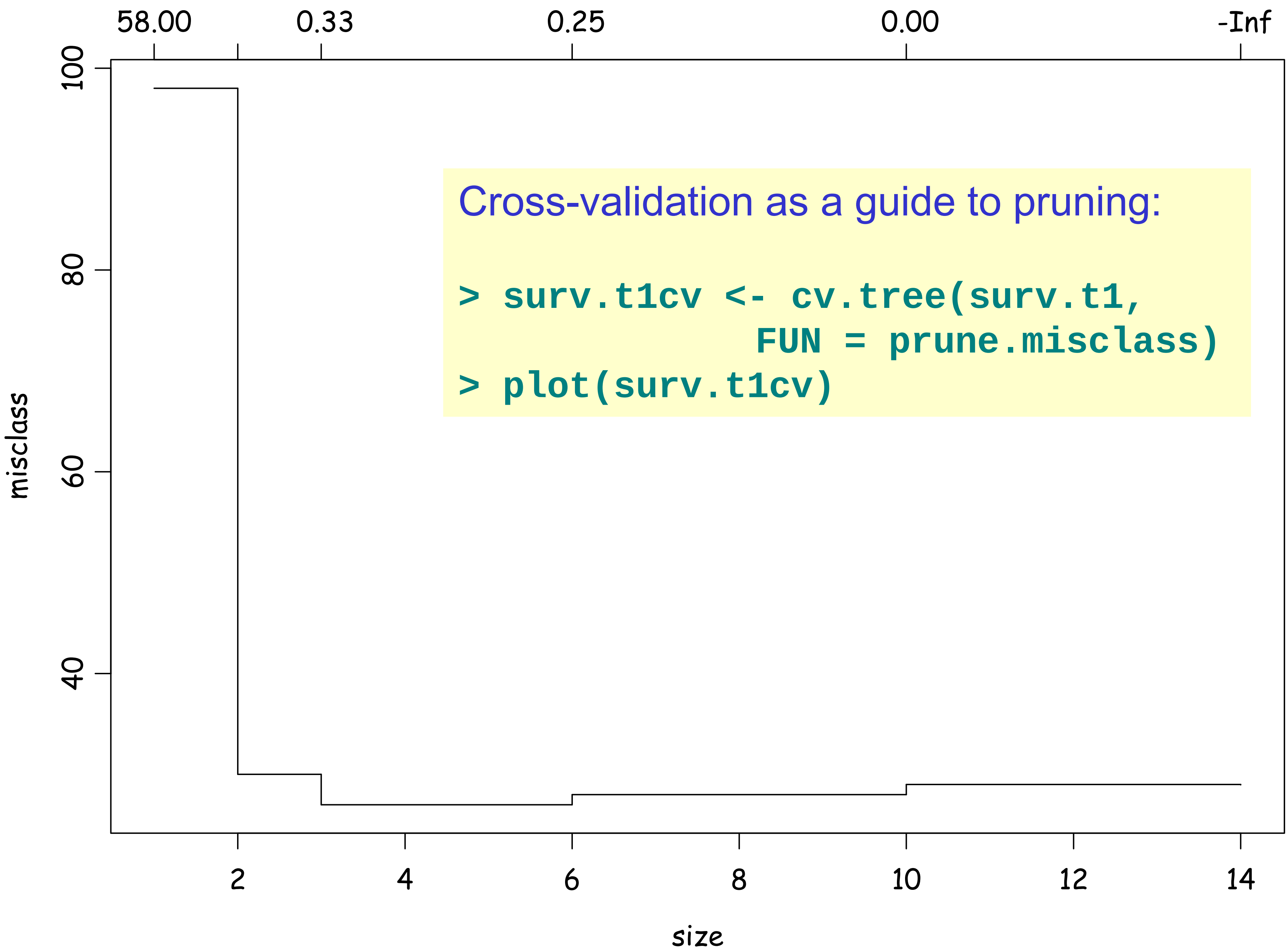
```
> obj <- cv.tree(tree.obj, FUN=functn, ...)

> plot(obj)
```

Currently `functn` must be either `prune.tree` or `shrink.tree` (the default). It determines the protocol by which the sequence of trees tested is generated. The MASS library also has `prune.misclass` for classification trees, only.

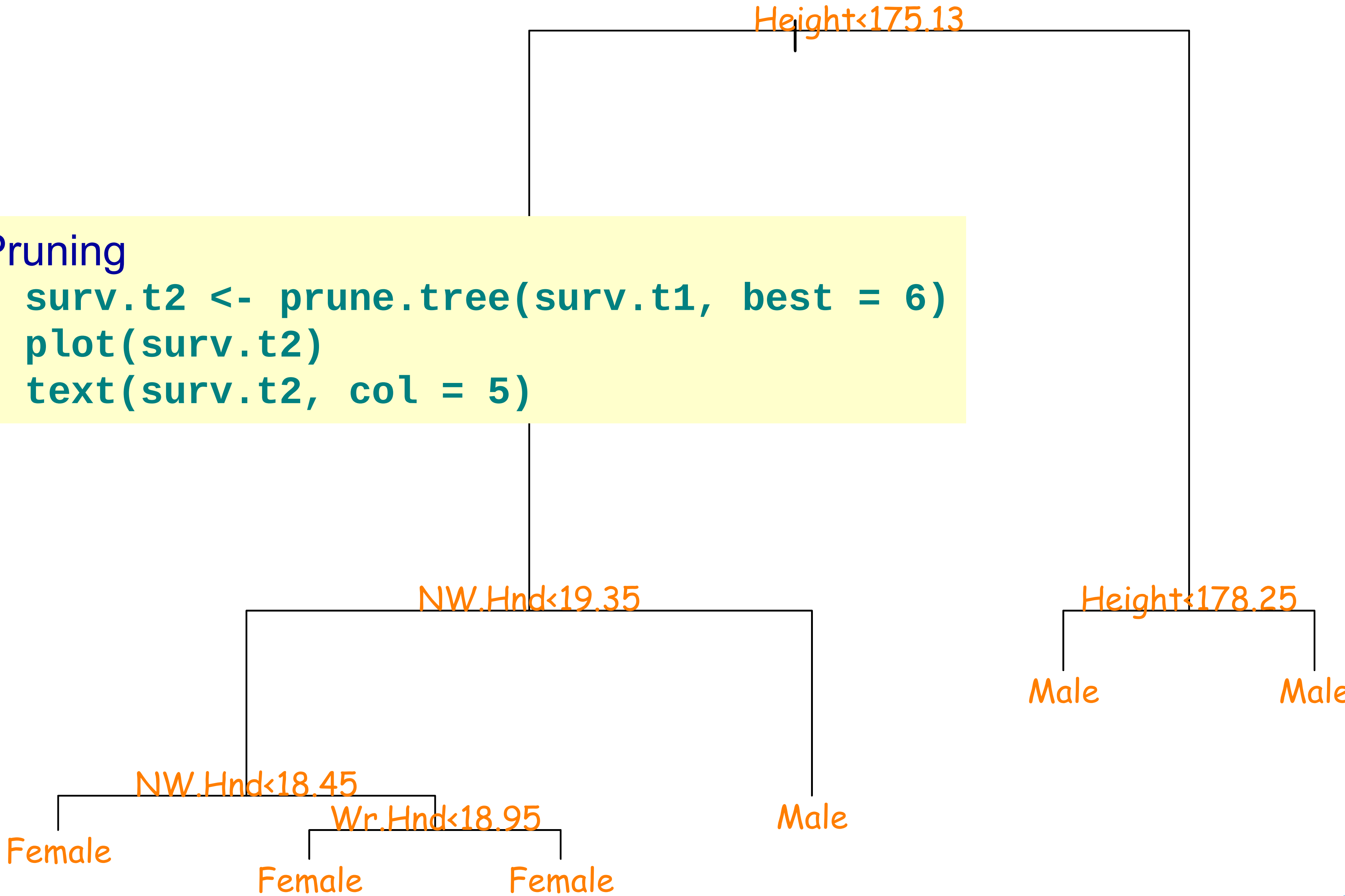
Cross-validation as a guide to pruning:

```
> surv.t1cv <- cv.tree(surv.t1,
                FUN = prune.misclass)
> plot(surv.t1cv)
```



Pruning

```
> surv.t2 <- prune.tree(surv.t1, best = 6)
> plot(surv.t2)
> text(surv.t2, col = 5)
```



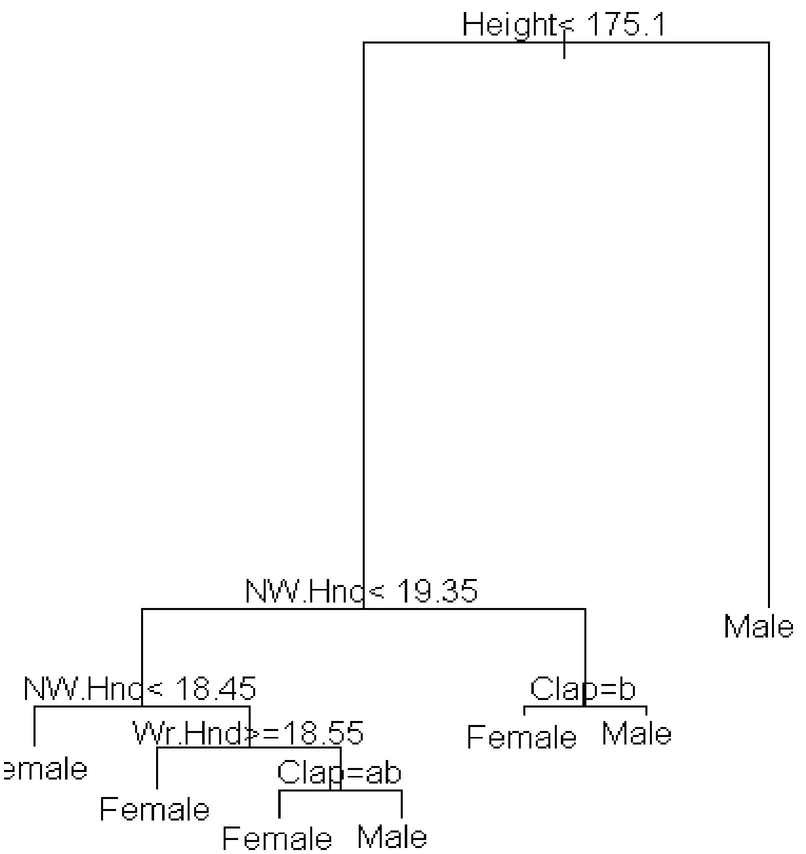
rpart counterpart

```
> rp1 <- rpart(Sex ~ ., Srvy,
               minsplit = 10)
> plot(rp1)
> text(rp1)
> plotcp(rp1)
```

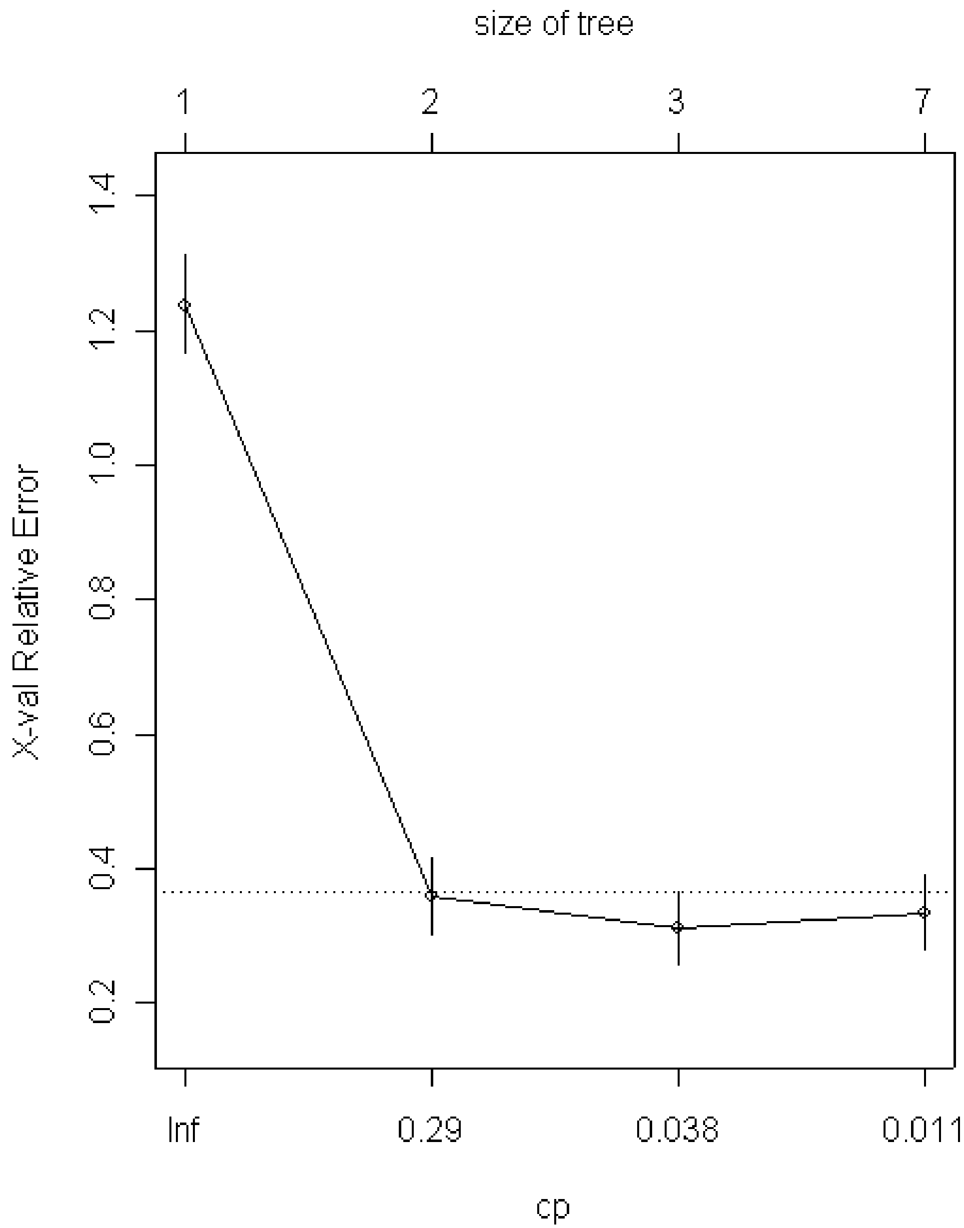
See next slide. This suggests a very small tree – two nodes. (Some repeat tests might be necessary.)

```
> rp2 <- prune(rp1, cp = 0.29)
> plot(rp2)
> text(rp2)
```

rpart tree with minsplit = 10



Internal cross-validation and the 'one se' rule



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Confusion matrices

- Now to check the effectiveness of the pruned tree on the training sample.
- Should be pretty good!

```
> table(predict(surv.t2, type = "class"),
                                 Srvy$Sex)
       Female Male
Female     79   11
  Male      5   73
```

- Next step: build on a training set, test on a test.

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First build the model.

```
> w <- sample(nrow(Srvy), nrow(Srvy)/2)
> Surv0 <- Srvy[w, ]
> Surv1 <- Srvy[-w, ]
> surv.t3 <- tree(Sex ~ ., Surv0)
```

Check on training set:

```
> table(predict(surv.t3, type="class"),
                                 Surv0$Sex)
       Female Male
Female     42    2
  Male      3   37
```

Test on test set:

```
> table(predict(surv.t3, Surv1, type="class"),
  Surv1$Sex)
       Female Male
Female     34    6
  Male      5   39
```

Now build an over-fitted model on the training set and check its performance:

```
> surv.t3 <- tree(Sex ~ ., Surv0, minsize = 4)
> table(predict(surv.t3, type="class"),
  Surv0$Sex)
         Female Male
Female       44    1
  Male        1   38
```

Far too good! How does it look on the test set?

```
> table(predict(surv.t3, Surv1, type="class"),
                                    Surv1$Sex)
         Female Male
Female       31    9
  Male        8   36
```

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Bagging requires fitting the same model a sequence of 'bootstrapped data frames'. It is convenient to have a function to do it.

```
> jig <- function(dataFrame)
      dataFrame[sample(nrow(dataFrame), rep = T),  ]
```

Now for the bagging itself

```
> bag <- list()
> for(i in 1:100)
      bag[[i]] <- update(surv.t3, data = jig(Surv0))
```

Next find the sequence of predictions for each model using the test set. It is convenient to have the result as characters.

```
> bag.pred <- lapply(bag, predict,
                 newdata = Surv1, type = "class")
> bag.pred <- lapply(bag.pred, as.character)
```

Finding the winner

Using a single call to `table()`, find the frequency of each prediction for each row of Surv1:

```
> tab <- table(rep(1:nrow(Surv1), 100), unlist(bag.pred))
```

Now find the maxima, avoiding any "one at a time" method.

```
> maxv <- tab[,1]
> maxp <- rep(1, nrow(tab))
> for(j in 2:ncol(tab)) {
      v <- maxv < tab[,j]
      if(any(v)) {
          maxv[v] <- tab[v, j]
          maxp[v] <- j
      }
  }
> table(levels(Surv1$Sex)[maxp], Surv1$Sex)
       Female Male
Female     36    7
  Male      3   38
```

Now 10 rather than 17 misclassifications.

Tree models: some pros and cons

- Tree based models are easy to appreciate and discuss. The important variables stand out. Non-additive and non-linear behaviour is automatically captured.
- Mixed factor and numeric variables are simply accommodated.
- The scale problem for the response is no worse than it is in the regression case.
- Linear dependence in the predictors is irrelevant, as are monotone transformations of predictors.

- Experience with the technique is still in its infancy. The theoretical basis is still very incomplete.
- Strongly coordinate dependent in the predictors.
- Unstable in general.
- Non-uniqueness. Two practitioners will often end up with different trees. This is not important if inference is not envisaged.