



ETC3580: Advanced Statistical Modelling

Week 1: Visualizing linear models

Outline

1 Linear Models Review

2 Linear models in R

3 Visualization

4 Interactions

5 Hypothesis testing

6 Variable selection

Linear Models

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + \varepsilon$$

- Response: y
- Predictors: x_1, \dots, x_p
- Error: $\varepsilon \sim \text{IID}$

Let $\mathbf{y} = (y_1, \dots, y_n)'$, $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_n)'$, $\boldsymbol{\beta} = (\beta_0, \dots, \beta_p)'$ and

$$\mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & x_{2,1} & \dots & x_{p,1} \\ 1 & x_{1,2} & x_{2,2} & \dots & x_{p,2} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{1,n} & x_{2,n} & \dots & x_{p,n} \end{bmatrix} \quad (\text{the model matrix}).$$

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Then

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

Matrix formulation

Least squares estimation

Minimize: $(\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta)$

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Differentiate wrt β gives

The “normal” equations

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

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So MLE = OLS.

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R modelling notation

```
fit <- lm(y ~ x1 + x2 + x3,  
          data=tibble)
```

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2)$$

```
## # A tibble: 200 x 4  
##           y      x1      x2      x3  
##   <dbl> <dbl> <dbl> <dbl>  
## 1  78.6  51.3  47.8   2.8  
## 2  19.4  76.6  37.8  1.05  
## 3  97.6  26.1  24.2  4.63  
## 4  81.5  21.6 -19.3  1.9
```

Useful helper functions

Base functions

- `summary`
- `coef`
- `fitted`
- `predict`
- `residuals`

broom functions

- `tidy`
- `augment`
- `glance`

R formulas

Categorical predictors:

- R will create the required dummy variables from a categorical *factor*.
- The first level is used as the reference category.
- Use `relevel` to change the reference category

Expression	Description
$y \sim x$	Simple regression
$y \sim 1 + x$	Explicit intercept
$y \sim -1 + x$	Through the origin
$y \sim x + I(x^2)$	Quadratic regression
$y \sim x1 + x2 + x3$	Multiple regression
$\text{sqrt}(y) \sim x + I(x^2)$	Transformed
$y \sim . -x1$	All variables except $x1$

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Partial residuals

$$\mathbf{r} = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}$$

denote residuals for a given model fit.

Then the partial residuals for variable j are given by

$$\mathbf{r}_j = \mathbf{y} - \mathbf{X}_{-j}\hat{\boldsymbol{\beta}}_{-j}$$

where the $-j$ subscript indicates the removal of the j th column/element.

- Equivalent to y adjusted for all variables other than x_j .
- Plotting \mathbf{r}_j vs \mathbf{x}_j shows the relationship of \mathbf{y} vs \mathbf{x}_j after adjustment.

Conditional plots

- Slope of regression of r_j on \mathbf{x}_j is β_j .
- Conditional plots show $r_j + \mathbf{x}_{-j|m}\beta_{-j}$ vs \mathbf{x}_j , where $\mathbf{x}_{-j|m}$ corresponds to median of numeric variables and mode for factors.
- Let \mathbf{x}^{*} denote row of design matrix constructed from $x_j = x$ and $\mathbf{x}_{-j|m}$. Then equation of line is $\mathbf{x}^{*'}\hat{\beta}$ and standard error at x is

$$se(x) = \sqrt{\mathbf{x}^{*'}\text{Var}(\hat{\beta})\mathbf{x}^*}.$$

- Construct confidence interval using

$$\mathbf{x}^{*'}\hat{\beta} \pm t_{n-p, 1-\alpha/2} se(x)$$

Visualization using visreg

- `visreg(ls_object)`
- `visreg(ls_object, "xvar", gg=TRUE)`

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Interactions occur when effect of one predictor on response changes with value of another predictor.

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- Plot y vs x_j for different values of x_k
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To see 2-way interactions after adjustment

- Plot r_j vs x_j for different values of x_k
- Plot r_k vs x_k for different values of x_j

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- Plot r_j vs x_j for different values of x_k
- Plot r_k vs x_k for different values of x_j

Much harder to see higher-order interactions

Interactions

Interactions:

- One possible type of interaction is obtained by multiplying the relevant columns of the model matrix.
- Use $a:b$ for the interaction between a and b .
- Use $a*b$ to mean $a + b + a:b$
- Need to specify explicit functions for other types of interaction. e.g., $I(a/b)$

Limited order interactions:

- Interactions up to 2nd order can be specified using the $^{\wedge}$ operator.
- $(a+b+c)^2$ is identical to $(a+b+c)*(a+b+c)$

Nested factors:

- $a + b \%in\% a$ expands to $a + a:b$

Interpretation

- Each coefficient gives effect of one unit increase of predictor on response variable, *holding all other variables constant*.
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Visualization using visreg

- `visreg2d(ls_object, "xvar1", "xvar2")`
- `visreg2d(ls_object, "xvar1", "xvar2", plot.type='persp')`
- `visreg2d(ls_object, "xvar1", "xvar2", plot.type='rgl')`
- `visreg2d(ls_object, "xvar1", "xvar2", plot.type='gg')`

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Hypothesis testing

- Use F-tests between models:
 - Model 1: p_1 parameters.
 - Model 2 (nested within Model 1): p_2 parameters

$$F = \frac{(RSS_2 - RSS_1)/(p_1 - p_2)}{RSS_1/(n - p_1)} \sim F_{p_1 - p_2, n - p_1}$$

- Helper functions: `anova`, `drop1`
- If one term dropped, this is equivalent to a t-test on coefficient.

Hypothesis testing

`anova(model)`

- provides sequential testing of terms (conditional on all previous terms)
- Order of terms will usually affect the p-values.
- Uses “Type 1” SS

`anova(model1, model2)`

- Tests two nested models.
- Avoids ordering problems

`drop1(model, test="F")`

- Equivalent to series of `anova(model1, model2)` calls where `model2` drops one variable at a time.
- Equivalent to “Type 3” SS

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Akaike's Information Criterion

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$$\text{AIC} = -2 \log L + 2q$$

where q is the number of parameters in the model.

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- For Gaussian errors:

$$L = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta)\right)$$

$$-2 \log L = n \log(2\pi\sigma^2) + \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta)$$

$$= c + \frac{\text{SSE}}{2\sigma^2}$$

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`extractAIC()` used by `step()`
handles c and q differently from `AIC()`

Variable selection

step() will minimize AIC using backwards selection

Best model with only main effects

```
mod1 <- lm(y ~ x1 + x2 + x3, data=data) %>%  
  step()
```

Best model with up to 2-way interactions

```
mod2 <- lm(y ~ (x1 + x2 + x3)^2, data=data) %>%  
  step()
```

Best model with up to 3-way interactions

```
mod3 <- lm(y ~ (x1 + x2 + x3)^3, data=data) %>%  
  step()
```

Variable selection and inference

- Do not use coefficient t-tests for variable selection.
- Beware of *any* statistical tests after variable selection.
- Confidence intervals after variable selection are too narrow.
- Variable selection is most useful for prediction. If you are only interested in inference, don't do it!