Index of Lecture 1b

Practical Information

Today's lecture: catch-up from Lecture 1a (backtransformation), and start of multiple linear regression,

- interpretation of models and parameters,
- comparing models by statistical tests, incl. special case: test of linearity for grouped continuous predictor.
- polynomial regression,
- new issue in multiple linear regression: collinearity,
  - ways to detect and deal with it,
  - examples from MER and RC (old VHM 802 text).[1]

Textbook reading:

- VER2: essentially same introductory pages as for first lecture plus Section 14.5 on collinearity,
- PSLS[2]: Suppl. Ch. 28 on Multiple & Logistic Regression.

Home work for Friday:

- Exercise 1 in "Linear Regression Exercises" (`btb-episodes` datasets at VHM 802 website and VHM 812 Moodle),
  - use your preferred statistical software for the calculations; solution files will be provided for Stata,
  - exercise review and Stata demo on Friday, followed by student work on more exercises (*bring your laptop!*).

[1] No good example in VER. The MER example expands on textbook coverage.
[2] *The Practice of Statistics in the Life Sciences*, 3rd ed.; the VHM 801 textbook.

Multiple Linear Regression Model

Dataset `daisy2red`: 1536 lactations of cows in multiple herds, focusing initially on the variables,

* y_i = milk yield during first 120 days (`milk120`),
* x_{1i} = parity (lactation number) (`parity`),
* x_{2i} = twin birth? (0=no/1=yes) (`twin`),
* x_{3i} = vaginal discharge? (0=no/1=yes) (`vag_disch`),[3]

for i^{th} lactation, $i = 1, \ldots, 1536$.

Purpose: use x-variables to predict milk yield (hoping that prediction will be valid, or meaningful, for wider population of lactations and cows).

Alternative purpose: examine "effect" of x-variables on milk yield (sign, strength, significance of effect), but because this is an observational study causal inference is not automatic (more in a later lecture).

Statistical model (with 3 predictors):

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \varepsilon_i,$$

where the errors $\varepsilon_1, \ldots, \varepsilon_{1536}$ are i.i.d. and $\sim \mathrm{N}(0, \sigma^2)$,

- "same" as simple linear regression, but more predictors,
- x's can be of multiple types (here: one continuous and two dichotomous predictors).

[3] After calving, vaginal discharge of certain types may serve as an indicator of different diseases/conditions for the cows, in particular metritis (urine infection).

Model Assumptions and Interpretations

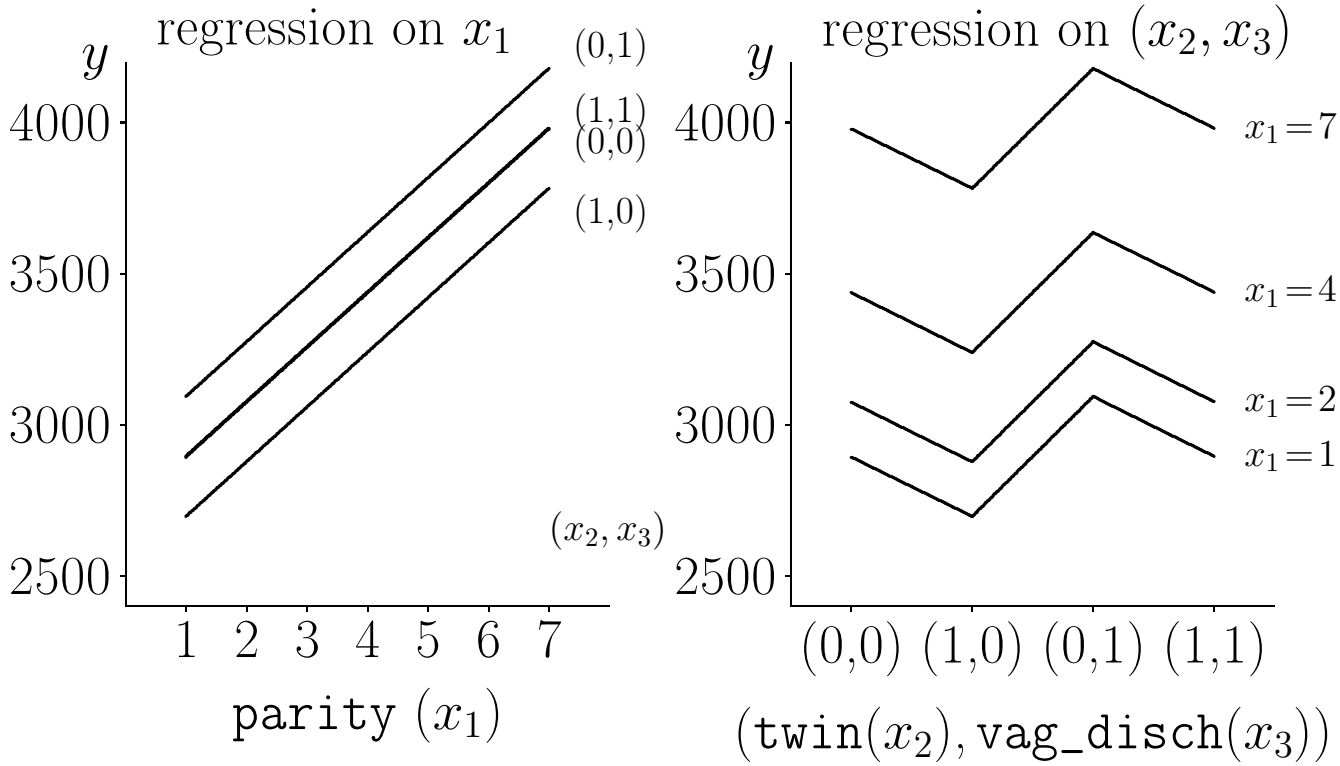
Model assumptions:

- independence, normality, variance homogeneity of ε_i's,
- linear relation:

$$\begin{aligned} \mathrm{E}(y_i) &= \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i}, \\ \hat{y} &= 2713.2 + 180.9\, x_1 + (-197.0)\, x_2 + 199.7\, x_3, \end{aligned}$$

  - $*$ *linear* "effect" of x_1 on y (for fixed x_2 and x_3),
  - $*$ *additive* "effects" of x_1, x_2 and x_3 (parallel curves in graphs (below), no interaction).

Fitted graphs of separate regressions (with other variable(s) fixed at the values indicated):



Multiple Linear Regression Analysis

Methods almost the same (as in simple linear regression):

- estimation by least squares method (minimising squared deviations between observed and predicted values),[4]
- confidence intervals, prediction and tests of simple hypotheses H_0: $\beta_i = 0$ using "4-step procedure",
  - prediction by same approach, but beware to avoid "outlying" sets of x-values: guideline: $\mathrm{SE}(\hat{y})/\sqrt{\mathrm{MSE}} \leq \sqrt{2(k+1)/n}$,
  - $\mathrm{DFE} = n-(k+1)$ (k = number of predictor parameters),
- analysis of variance (ANOVA) table:
  - F-test is for hypothesis H_0: all $\beta_j = 0$ (except β_0), against alternative H_a: some $\beta_j \neq 0$ (not necessarily all),[5]
  - $r^2(R^2) = \mathrm{SSM}/\mathrm{SST} \sim$ proportion of variance explained by model, or squared correlation between observed and *fitted* values.

New issues and interpretations:

- individual regression coefficients:
  - "effects" must be viewed/interpreted in presence of other predictors — and usually change if model changes (substantial changes in the presence of *collinearity*; later this lecture),
  - for example, proper interpretation for β_2:
    - ∼ "effect" of `twin` when x_1 and x_3 have been accounted for, (or when adding `twin` to model with x_1 and x_3),
    - ∼ difference in predictions between two identical lactations, except that one has `twin=1` and the other `twin=0`.
- variable selection to arrive at most succint model (Lectures 2a/3a).

[4] Closed formulae exist but involve matrix calculus (manual calc. infeasible).

[5] Note that F-test no longer corresponds to t-tests for individual β's.

Comparison of Models

Problem (example): does the reduced (R) model give an equally good data description as the full (F) model?

$$\begin{aligned}(\mathrm{R}):\ y_i &= \beta_0 + \beta_1\, x_{1i} + \varepsilon_i,\\ (\mathrm{F}):\ y_i &= \beta_0 + \beta_1\, x_{1i} + \beta_2\, x_{2i} + \beta_3\, x_{3i} + \varepsilon_i.\end{aligned}$$

Idea: use statistical test to compare two models, *if one model is a submodel of the other one*:

- compute residual sum of squares for models (F),(R): $\mathrm{SSE(F)} \le \mathrm{SSE(R)}$, (more parameters $\Rightarrow$ better fit)
- compute residual degrees of freedom for models (F),(R): $\mathrm{DFE(F)} \le \mathrm{DFE(R)}$, (more parameters $\Rightarrow$ less DF)
- compute test statistic:

$$\begin{aligned}F &= \frac{[\mathrm{SSE(R)} - \mathrm{SSE(F)}]/[\mathrm{DFE(R)} - \mathrm{DFE(F)}]}{\mathrm{MSE(F)}}\\ &\sim F\big(\mathrm{DFE(R)} - \mathrm{DFE(F)}, \mathrm{DFE(F)}\big) \ \text{ under } \mathrm{H_0}\text{: model (R)},\end{aligned}$$

  alternatively, $\mathrm{H_0}$ may be expressed that $\beta_i = 0$ for all variables removed from model (F) to model (R).
- example: $F = \frac{[638\,905\,966 - 635\,235\,472]/[1534-1532]}{414\,645} = 4.43$ $\sim P = 0.012$ in $F(2, 1532)$ $\Rightarrow$ model (R) is insufficient.

Alternative approach: test removal of extra β's in model (F) one at a time,

- several tests instead of one (same conclusions?),
- necessary to fit several models between (F) and (R).

More Model Comparisons

VER Example 14.3: model with additional predictors:

- x_{4i} = dystocia (difficult calving)? (0=no/1=yes) (`dyst`),
- x_{5i} = retained placenta? (0=no/1=yes) (`rp`),
- (for simplicity) $\tilde{y}_i$ = milk yield in 1000s (`milk120/1000`).

Model schematic:

5-predictor multiple regression $y_i = \beta_0 + \beta_1 x_{1i} + \ldots + \beta_5 x_{5i} + \varepsilon_i$	SSE= DFE=

3-predictor multiple regression $y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \varepsilon_i$	SSE=635.235 DFE=1532

$\downarrow$ $F = 4.43$ $(P = 0.01)$

Simple linear regression $y_i = \beta_0 + \beta_1 x_{1i} + \varepsilon_{ij}$	SSE=638.906 DFE=1534

One sample $y_i = \beta_0 + \varepsilon_i$	SSE= DFE=

Polynomial Regression

Statistical model:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \ldots + \beta_k x_i^k + \varepsilon_i,$$

where the errors $\varepsilon_1, \ldots, \varepsilon_n$ are assumed i.i.d. and $\sim \mathrm{N}(0, \sigma^2)$.

Special cases:

$k = 1$ (linear regression): $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$,
$k = 2$ (quadratic regr.): $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i$,
$k = 3$ (cubic regression): $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \varepsilon_i$.

Interpretation of parameters:

- quadratic model: added curvature (β_2),
- cubic model: added "bump" (β_3),
- always: $\beta_0 \sim$ intercept (value for $x = 0$),
- parameters $\beta_1, \ldots, \beta_{k-1}$ in k^{th} order model have *no useful interpretation*, but should be kept in model!

Polynomial regression modelling:

- low order polynomials most useful! (k at most 3 or 4),
- polynomials may give poor predictions outside and in special cases also inside (!) range of x's,
- test of linearity: add quadratic term, and test H_0: $\beta_2 = 0$,
- often no physical/biological meaning, but easy to analyse because a linear model, despite the non-linear relation.[6]

[6] As discussed in footnote 6 on page L1a−7.

Quadratic Regression Equation

daisy2red data example:

$$\texttt{milk120}_i = \beta_0 + \beta_1 \texttt{parity}_i + \beta_2 \texttt{parity}_i^2 + \varepsilon_i,$$

with the errors $\varepsilon_1, \ldots, \varepsilon_{1536}$ assumed i.i.d. and $\sim \mathrm{N}(0, \sigma^2)$.

Interpretation:

- fitted regression curve by least squares estimation:

  $$\texttt{milk120} = 2109 + 697.50\,\texttt{parity} - 82.557\,\texttt{parity}^2,$$

  – for prediction *within the data range* of parities;
  the best representation of the model is by a graph of $\hat{y}$ against x for a sensible range of x-values,
- intercept $= 2109 \sim$ value for $\texttt{parity} = 0$ (meaningless!),
- curvature $= \hat{\beta}_2 = -82.557$ ($< 0 \sim$ "sad" parabola),
  H_0: $\beta_2 = 0 \sim$ no curvature (hence a linear relation),
- linear component $= \hat{\beta}_1$: no useful interpretation!
  H_0: $\beta_1 = 0 \sim$ parabola centred at $\texttt{parity} = 0$ (meaningless),
  - problem is that the variables x and x^2 are highly *collinear* ("similar"; see later in lecture); e.g., changing x_1 while keeping x_2 fixed is impossible!,
  - (technical) best way to get interpretable coefficients is to reformulate model using *orthogonal polynomials*[7], but usually not considered worth the trouble...

[7] Stata command: `orthpoly`.

Quadratic Regression ANOVA

Source of variation	Sum of squares	Degrees of freedom	Mean square	F
Regression Model Error	 SSM SSE	 DFM$=2$ DFE$=n-3$	 MSM$=$SSM$/2$ MSE$=$SSE$/$DFE	 MSM$/$MSE
Total	SST	DFT$=n-1$		

- estimated error variance$=s^2=$ MSE (as usual), and $s=$ estimated standard deviation about regression curve,
- error degrees of freedom$=n-3$ (because of 3 estimated parameters) $\Rightarrow$ reference distribution is $t(n-3)$,
- F-test of hypothesis H_0: $\beta_1=0$ and $\beta_2=0 \sim$ no association (linear or quadratic) between y and x,
  - even if significant, the hypothesis H_0: $\beta_2=0$ is of interest (use 4-step approach),
- $r^2(R^2)=$ SSM$/$SST $=$ proportion explained by the model out of the total variation,
  - measure of predictive power of model (but *not* of model adequacy),
  - $=$ the squared correlation between y (observed values) and $\hat{y}$ (fitted values).

1-Way ANOVA with Quantitative Groups

`daisy2red` data example: parity as a grouping variable $\sim$ 1-way ANOVA model:[8]

$$\tilde{y}_i = \mu_{\text{parity}(i)} + \varepsilon_i, \quad i = 1, \ldots, 1536,$$

where $\mu_1, \mu_2, \ldots, \mu_7$ are the mean 120-day milk yields (in 1000s) for lactations of parity 1,. . . ,7, respectively.

2 candidate linear models: 1-way ANOVA and linear regression, with some links:

- test of linear regression against 1-way ANOVA,
- 1-way ANOVA $\equiv (a-1)$'th order regression, where a is the number of groups ($a = 7$ in example).

ANOVA tables:

(F): $\tilde{y}_i = \mu_{\text{parity}(i)} + \varepsilon_i$					(R): $\tilde{y}_i = \beta_0 + \beta_1 x_i + \varepsilon_i$				
Source	SS	DF	MS	F	Source	SS	DF	MS	F
Groups	184.64	6	30.77	83.5	Lin. reg.	109.23	1	109.2	262
Error	563.50	1529	.3685		Error	638.91	1534	.4165	
Total	748.14	1535			Total	748.14	1535		

Test of linear regression (or *lack of fit*):

= submodel (R) of 1-way ANOVA $\sim$ full model (F),

- usual F-statistic: $F = \frac{[638.91-563.50]/[1534-1529]}{.3685} = 40.9$,
  $\sim P \ll 0.001$ in $F(5, 1529)$ for linear regression model,
  $\Rightarrow$ very strong significance against the linear relation.

[8] Standard (incl. VHM 801) model notation: $y_{ij} = \mu_i + \varepsilon_{ij}$, with $i \sim$ groups.

Collinearity

* means that the different x-variables ($x_1, x_2, \ldots$) in multiple regression are similar (technically: non-orthogonal),
* is indicated by non-zero (partial) correlations among (continuous) x's; extreme corr. $\Rightarrow$ severe collinearity,
* is indicated also by Variance Inflation Factors[9] (VIFs) much greater than 1 ($\geq 5-10$ is "critical"),
* manifests itself as correlated parameter estimates.

Implications of collinearity:

- intuitively: difficult to separate/distinguish "effects" of collinear variables (they explain the "same thing"),
- each parameter's *estimate, test, amount of variance explained* depend (strongly) on *all* predictors in model,
- two non-significant t-tests for two variables in a model, do *not!* imply *both* to be redundant,
- also loss of precision on estimates (i.e., variance inflation).

Data example: effects of `cig_3` (x_3) in `bw5k` data (MER) for different models for birthweight (`bwt`; y) when also `cig_1`,`cig_2` (x_1, x_2) are included,

– regr. of y on x_3: $\hat{\beta}_3 = -12.5\,(2.6)$, $P < .0005$,

– regr. of y on x_1, x_3: $\hat{\beta}_3 = -6.5\,(4.8)$, $P = 0.17$,

– regr. of y on x_2, x_3: $\hat{\beta}_3 = -0.1\,(8.0)$, $P = 0.99$.

[9] In Stata, use `estat vif` to display VIFs after `regress`.

Correlated Parameter Estimates

Correlations between two random variables:

- recall that: $-1 \leq$ correlation ≤ 1,
- independence $\sim$ zero correlation,
- positive (negative) association $\sim$ positive (negative) corr.,
- simple example: linear regression slope and intercept estimates *negatively correlated* when x's away from zero,
- implication (in general): change in one variable affects other variable.

Correlations between regression parameter estimates:

- "rule": only values outside $(-0.5, 0.5)$ deserve attention,
- strong correlations with intercept are "normal",
- 2 strongly correlated parameter estimates cannot be interpreted independently, for example: removing one variable will affect the other one,
- many strongly correlated parameters: indication of an overfitted model (unrealistic good fit to data),
- (technical) related to the *partial correlation coefficients* between the x's.

How to compute correlations (between parameter estimates)?

- use suitable software tools after model has been fitted.[10]

[10] In Stata, use `vce,corr` command (or post-estimation menu).

Collinearity Example in RC

Data: from 20 schools in USA (Coleman report),

* y_i = mean verbal test score (6^{th} graders),
* x_{1i} = staff salaries per pupil,
* x_{2i} = percent of fathers with white collar jobs,
* x_{3i} = socioeconomic status,
* x_{4i} = mean verbal test score for *teachers*,
* x_{5i} = mean educational level for mothers,

for i^{th} school, $i = 1, \ldots, 20$.

Full regression model:

$$y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \varepsilon_i.$$

Exploration of collinearity (full regression model)

- correlations among the x-variables:
  strong correlations (> 0.8) between x_2, x_3 and x_5,
- variance inflation factors in full regression model:
  8.40 for x_2, 7.77 for x_5 and < 5 for other predictors,
- correlated parameter estimates in full regression model:
  $\text{Corr}(\hat{\beta}_2, \hat{\beta}_5) = -0.78$, all others (numerically) less than 0.5.

Collinearity Example (cont)

Parameter estimates in selected models:
(underlined estimates are significantly diff. from zero, or close)

Model	$\hat{\beta}_0$	$\hat{\beta}_1$	$\hat{\beta}_2$	$\hat{\beta}_3$	$\hat{\beta}_4$	$\hat{\beta}_5$	VIF[a]	Corr[b]
$x_1 - x_5$	19.9	-1.79	0.044	0.56	1.11	-1.81	8.4	-0.78
$x_1 - x_4$	11.5	-1.76	0.007	0.54	1.05	–	3.4	-0.83
$x_1, x_3 - x_5$	15.5	-1.71	–	0.58	1.03	-0.52	3.1	-0.82
x_1, x_3, x_4	12.1	-1.74	–	0.55	1.04	–	1.4	-0.23
x_3, x_4	14.6	–	–	0.54	0.75	–	1.0	-0.18
x_1	28.4	2.46	–	–	–	–	–	–
x_2	28.2	–	0.17	–	–	–	–	–
x_3	33.3	–	–	0.56	–	–	–	–
x_4	-2.0	–	–	–	1.48	–	–	–
x_5	-5.7	–	–	–	–	6.52	–	–
x_2, x_3, x_5	39.4	–	0.01	0.59	–	-1.06	7.9	-0.77

[a] maximal variance inflation factor among predictors in model
[b] strongest correlation among regression coefficients (excl. $\hat{\beta}_0$) in model

Conclusions/Findings:

- very variable intercepts (not too surprising),
- effect of x_3 remarkably constant,
- effects of x_2 and x_5 quite variable and significant on their own but not in combination with x_3,
- effect of x_4 only significant in combination with x_3,
- strong correlations may appear in reduced models (e.g., $x_1 - x_4$),
- correlations can be high quite high even if VIFs are low.

Summary: Collinearity

Strong collinearity between predictors/parameters (excluding the intercept) is a problem,

i) for interpretation of estimates,[11]

ii) possibly also for the estimation itself (extreme cases).

and should then be *avoided* by omitting or combining the predictors involved.

Note: strong collinearity occurs "naturally" in some situations:

- between linear and quadratic terms of x (generally, between polynomial terms),
- between main effect and interaction terms,
- between indicator (dummy) variables representing a categorical predictor (next lecture),

because the variables involved are truly related...; in these instances, collinearity would only be a real problem for reason *ii)*.

For collinearity involving quantitative predictors and its derived variables (quadratic or interaction terms), collinearity may be reduced by a technique called "centring":

- replacing x by $(x - \bar{x})$ in the model equation,
- not affecting model fit or predictions.

The main advantage of "centring" is improved interpretation of parameters, discussed in the next lecture.[12]

[11] Also important for interpretation is the related issue of confounding between predictors in epidemiological studies (next lecture); generally speaking, strong confounding can only occur when (strong) collinearity exists.

[12] Example 14.8 in VER demonstrates how "centring" may reduce collinearity, but this would only be of real interest if VIFs were needed to detect other collinearities.