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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,
- PSLS²: Suppl. Ch. 28 on Multiple & Logistic Regression.

Home work for Tuesday:

- 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 and Minitab (any interest in other packages?),
 - * exercise review and detailed Stata demo on Tuesday.

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, $i = 1, \dots, 1536$.

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

Alternative purpose: examine “effect” of x -variables on milk yields (sign, strength, significance of effects), but observational study so 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 $\varepsilon_1, \dots, \varepsilon_{1536}$ are i.i.d. and $\sim N(0, \sigma^2)$,

- “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 serve as indicator of different diseases/conditions for the cows, in particular metritis (urine infection).

MODEL ASSUMPTIONS AND INTERPRETATIONS

Model assumptions:

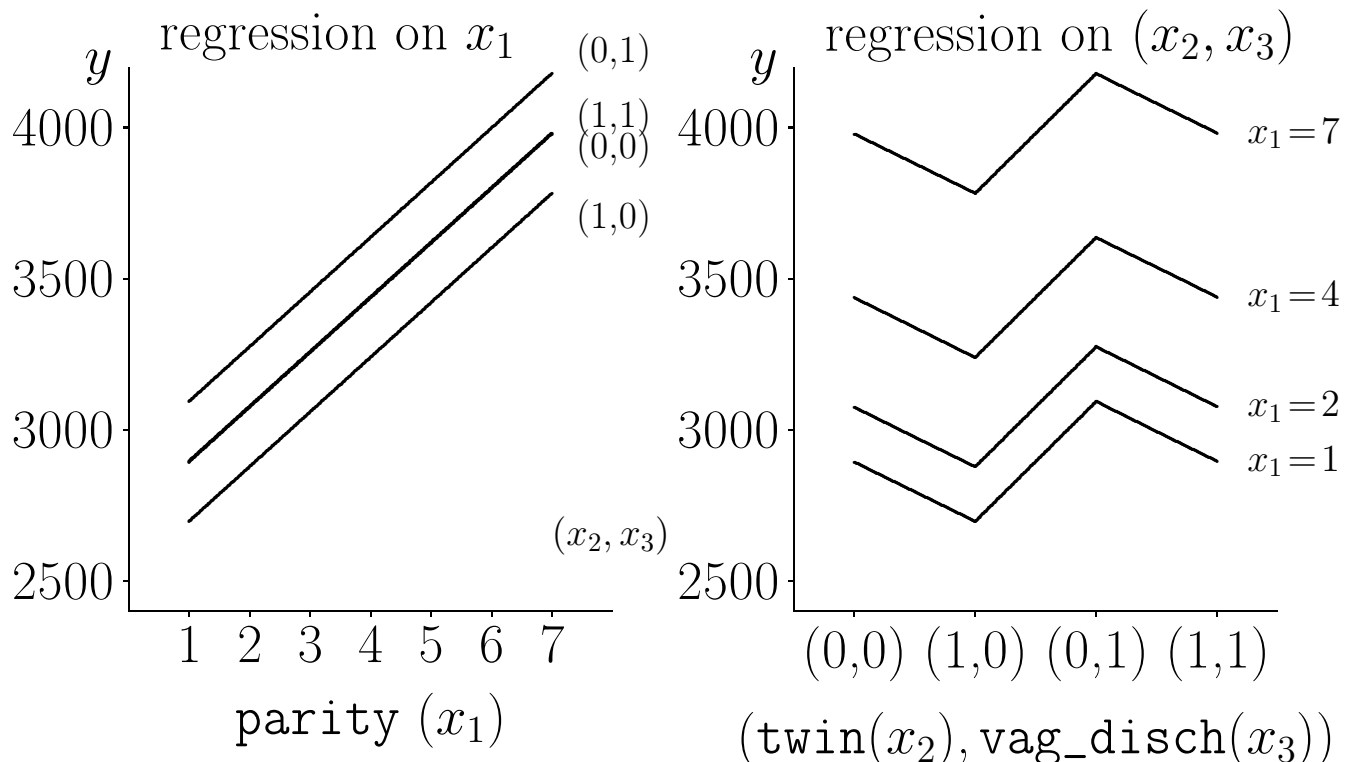
- independence, normality, variance homogeneity of ε_i 's,
- linear relation:

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

$$\hat{y} = 2713 + 180.9 x_1 + (-197.0) x_2 + 199.7 x_3,$$

- * *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: $SE(\hat{y})/\sqrt{MSE} \leq \sqrt{2(k+1)/n}$,
- $DFE = n - (k + 1)$ ($k =$ number of predictor parameters),
- analysis of variance (ANOVA) table:
 - * F -test is for hypothesis $H_0: \text{all } \beta_j = 0$ (except β_0), against alternative $H_a: \text{some } \beta_j \neq 0$ (not necessarily all),⁵
 - * $r^2(R^2) = SSM/SST \sim$ 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 :
 - \sim “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),
 - \sim difference in predictions between two identical lactations, except that one has **twin=1** and the other **twin=0**.
- variable selection to arrive at most succinct 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?

$$(R) : y_i = \beta_0 + \beta_1 x_{1i} + \varepsilon_i,$$

$$(F) : y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \varepsilon_i.$$

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):
 $SSE(F) \leq SSE(R)$, (more parameters \Rightarrow better fit)
- compute residual degrees of freedom for models (F),(R):
 $DFE(F) \leq DFE(R)$, (more parameters \Rightarrow less DF)
- compute test statistic:

$$F = \frac{[SSE(R) - SSE(F)] / [DFE(R) - DFE(F)]}{MSE(F)}$$

$\sim F(DFE(R) - DFE(F), DFE(F))$ under H_0 : model (R),
 alternatively, 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,

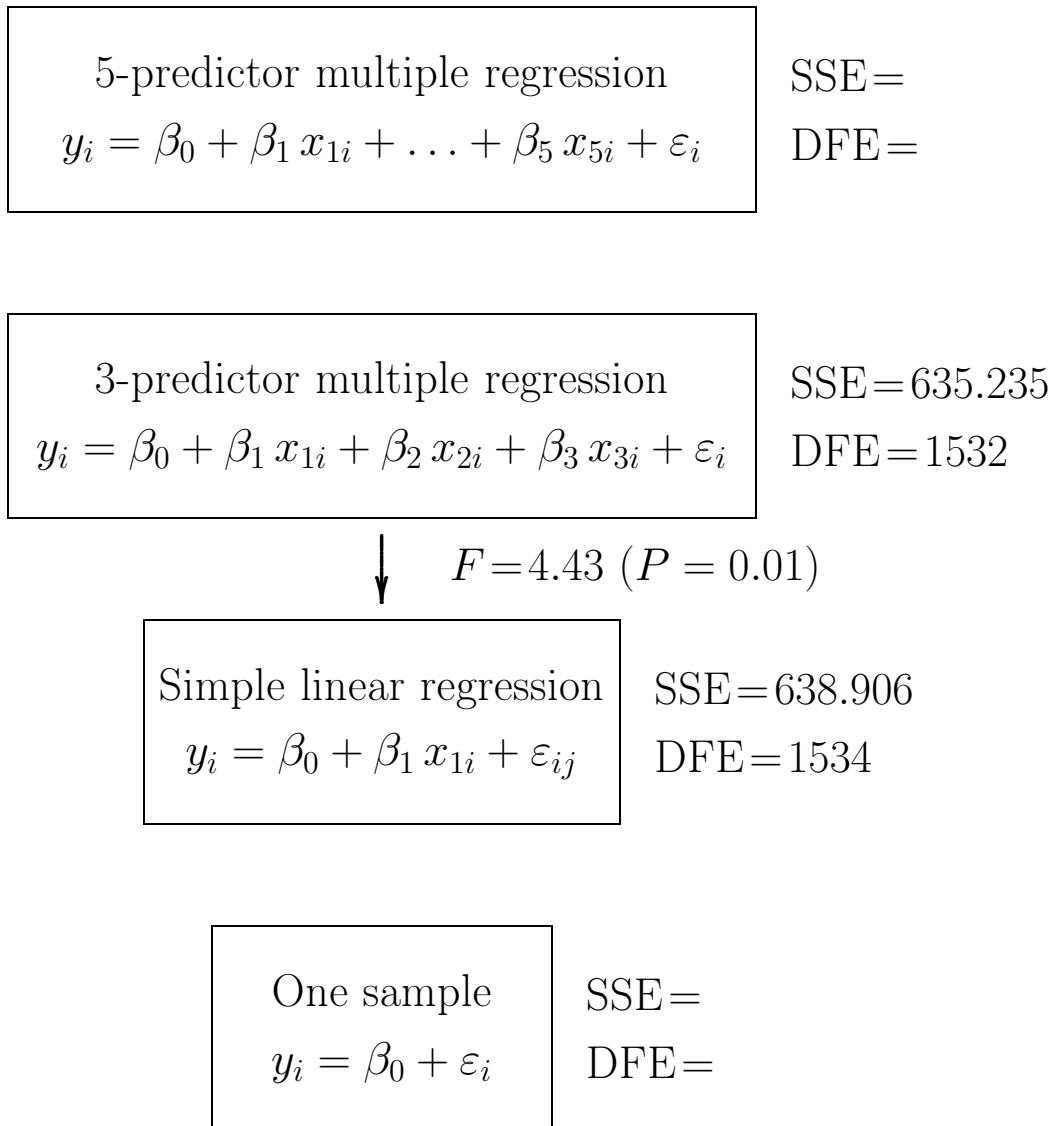
- several tests instead of one (same conclusions?),
- involves fitting several models between (F) and (R).

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:



POLYNOMIAL REGRESSION

Statistical model:

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

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

Special cases:

$$k = 1 \text{ (linear regression): } y_i = \beta_0 + \beta_1 x_i + \varepsilon_i,$$

$$k = 2 \text{ (quadratic regr.): } y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i,$$

$$k = 3 \text{ (cubic regression): } y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \varepsilon_i.$$

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 $\beta_1, \dots, \beta_{k-1}$ 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.

QUADRATIC REGRESSION EQUATION

daisy2red data example:

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

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

Interpretation:

- fitted regression curve by least squares estimation:

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

– 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 $\text{parity} = 0$ (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 $\text{parity} = 0$ (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*, but usually not considered worth the trouble...

QUADRATIC REGRESSION ANOVA

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

- estimated error variance = $s^2 = \text{MSE}$ (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),
- $r^2(R^2) = \text{SSM}/\text{SST} =$ 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:⁶

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

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

2 candidate 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.

⁶ 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, \dots) 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 Factors⁷ (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 : $\hat{\beta}_3 = -0.1 (8.0)$, $P = 0.99$.

⁷ In Stata, use `estat vif`.

CORRELATED PARAMETER ESTIMATES

Correlations between two random variables:

- recall that: $-1 \leq \text{correlation} \leq 1$,
- 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.⁸

⁸ In Stata, use: `estat vce, corr`; in Minitab, use macros.

COLLINEARITY EXAMPLE IN RC

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

- * y_i = mean verbal test score (6th 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, $i = 1, \dots, 20$.

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 ¹	Corr ²
$x_1 - x_5$	19.9	-1.79	0.044	<u>0.56</u>	<u>1.11</u>	-1.81	8.4	-0.78
$x_1 - x_4$	11.5	-1.76	0.007	<u>0.54</u>	<u>1.05</u>	–	3.4	-0.83
$x_1, x_3 - x_5$	15.5	-1.71	–	<u>0.58</u>	<u>1.03</u>	-0.52	3.1	-0.82
x_1, x_3, x_4	12.1	-1.74	–	<u>0.55</u>	<u>1.04</u>	–	1.4	-0.23
x_3, x_4	14.6	–	–	<u>0.54</u>	<u>0.75</u>	–	1.0	-0.18
x_1	28.4	2.46	–	–	–	–	–	–
x_2	28.2	–	<u>0.17</u>	–	–	–	–	–
x_3	33.3	–	–	<u>0.56</u>	–	–	–	–
x_4	-2.0	–	–	–	1.48	–	–	–
x_5	-5.7	–	–	–	–	<u>6.52</u>	–	–
x_2, x_3, x_5	39.4	–	0.01	<u>0.59</u>	–	-1.06	7.9	-0.77

¹ maximal variance inflation factor among predictors in model

² strongest correlation among regression coefficients (excl. $\hat{\beta}_0$) in model

Conclusions/Observations:

- 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,⁹

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...; then, collinearity is only 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.¹⁰

⁹ 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.

¹⁰ 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.