Epidemiology/Biostats VHM 812/802 Course
Winter 2014, Atlantic Veterinary College, PEI
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Index of Lecture 1b

PRACTICAL INFORMATION

Today's lecture: 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,
- IPS[2]: Chapter 11 on Multiple Linear Regression is an easy-to-read introduction to multiple linear 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, Minitab, SAS and R,
  - ∗ exercise review and detailed Stata demo on Tuesday.

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[1] No good example in VER. The MER example expands on textbook coverage.

[2] *Introduction to the Practice of Statistics* Eds. 6/7; the textbook for VHM 801.

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 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 $\varepsilon_1, \ldots, \varepsilon_{1536}$ 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).

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[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

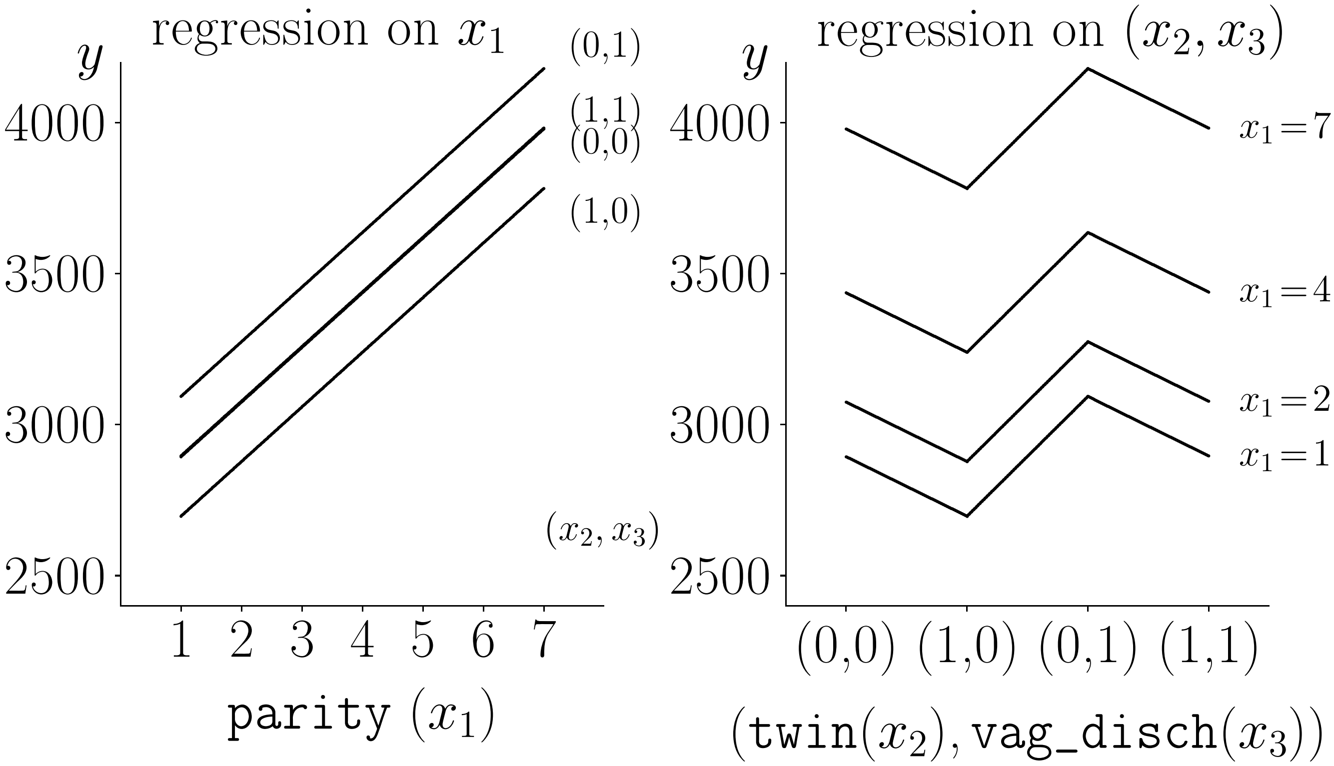
Model assumptions:

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

$$\begin{aligned} \mathrm{E}(y_i) &= \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i}, \\ \hat{y} &= 2713 + 180.9\, x_1 + (-197.0)\, x_2 + 199.7\, x_3, \end{aligned}$$

  - ∗ *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 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: $\mathrm{SE}(\hat{y})/\sqrt{\mathrm{MSE}} \leq \sqrt{2(k+1)/n}$,
- 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]
  - $*$ $R^2 = \mathrm{SSM}/\mathrm{SST} \sim$ 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*; L1b−11f),
  - $*$ 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 succint model (lectures 2a/3a).

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[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): $\mathrm{SSE(F)} \leq \mathrm{SSE(R)}$, (more parameters $\Rightarrow$ better fit)
- compute residual degrees of freedom for models (F),(R): $\mathrm{DFE(F)} \leq \mathrm{DFE(R)}$, (more parameters $\Rightarrow$ less DF)
- compute test statistic:
  $$F = \frac{[\mathrm{SSE(R)}-\mathrm{SSE(F)}]/[\mathrm{DFE(R)}-\mathrm{DFE(F)}]}{\mathrm{MSE(F)}}$$
  $$\sim F(\mathrm{DFE(R)}-\mathrm{DFE(F)}, \mathrm{DFE(F)}) \ \text{ under } \mathrm{H}_0\text{: model (R)},$$
  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 $F(2, 1534)$ $\Rightarrow$ 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:

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

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

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,
- non-linear relation but still a linear model.

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 `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 `parity`$=0$ (meaningless),
  - ∗ problem is that the variables x and x^2 are highly *collinear* (similar; see L1b–11f); 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$=s^2$ = MSE (as usual), and s = estimated standard deviation about regression curve,
- error degrees of freedom$=n-3$ (because of 3 estimated parameters) ⇒ reference distribution is $t(n-3)$,
- F-test of hypothesis H$_0$: $\beta_1=0$ and $\beta_2=0$ ∼ 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 ∼ 1-way ANOVA model:[6]

$$\tilde{y}_i = \mu_{\text{parity}(i)} + \varepsilon_i, \quad i = 1, \ldots, 1534,$$

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 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 ∼ 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, ⇒ very strong significance against the linear relation.

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

COLLINEARITY

- $*$ means that the different x-variables ($x_1, x_2, \ldots$) 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 (`vif` in Stata) 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 (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: $\hat{\beta}_3 = -0.1\,(8.0)$, $P = 0.99$.

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 (Stata: `estat vce`) after model has been fitted.

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

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

and should 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.[7]

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[7] 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.