Index of Lecture 1a

Introduction to Regression

Linear regression – in a broad sense:

- defining feature: error terms ∼ normal distribution,
- one or several predictors (independent or x-variables),
- predictors of all types (continuous, dichotomous, ordinal, nominal)
  ⇒ includes (e.g.) two-sample and ANOVA-type models,

– usually termed Linear Models[1].

Today's lecture:

- review of simple linear regression, expanding on model checking tools that *apply generally* to linear models,
- transformation, in particular power transformation and the Box-Cox method for selecting a transformation – also applies generally to linear models,
- computer-assisted using Stata.

Textbook reading:

- VER: 14.1–3 + 14.8–10 deal with multiple regression,
- GO: model checking procedures in Chapter 6 discussed in terms of a 1-way ANOVA.

Notation of lecture(s) mainly follows GO, e.g. variables (e.g., x and y) are not capitalized.

[1] Sometimes General Linear Models, e.g. in Minitab and SAS software.

Dataset `DAISY2`

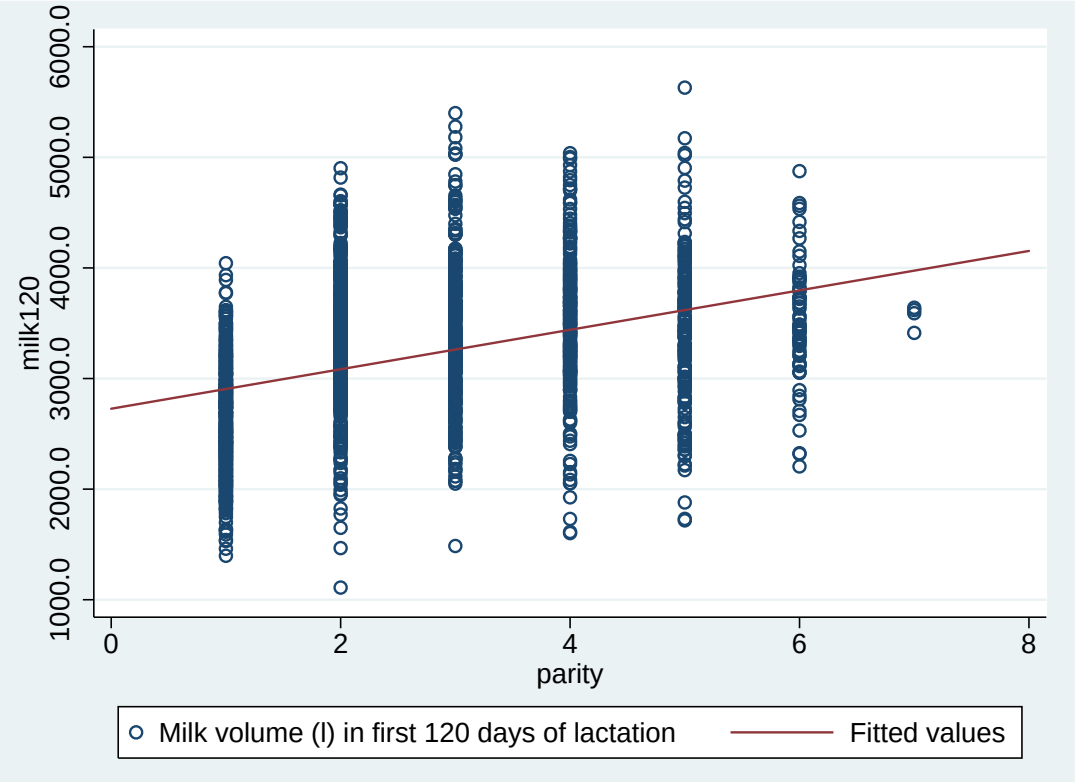
- VER2 dataset (from VER website),[2]
- real data $\sim$ single cohort study involving more than 8000 cows in 42 herds,
- contributed by John Morton, Australia,
- purpose of study: evaluate the effect of various diseases on milk yield and reproductive performance,
- focus here (entire VER Ch. 14) on subdataset (`daisy2red`) from 7 herds with high rates of reproductive diseases (1574 lactations from 1446 cows):

Variable	Description	Values
herd	herd number	(nominal)
cow	cow number	(nominal)
parity	lactation number	1–7
milk120*	milk volume in first 120 days of lact.	1110–5630 l
wpc	wait period to conception interval	1–298 days
twin	twin birth?	0/1
dyst	dystocia at calving?	0/1
vag_disch	vaginal discharge observed?	0/1
rp	retained placenta at calving?	0/1
herd_size	herd size	125–333
calv_dt	calving date	(date)

* 38 missing values

[2] Datasets are available at VHM 802 Exercises page (multiple formats).

Simple Linear Regression – Model



Statistical model:

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad i = 1, \ldots, 1536 \sim \text{ lactations},$$

where the errors $\varepsilon_1, \ldots, \varepsilon_{1536}$ are i.i.d.[3] and $\sim \mathrm{N}(0, \sigma^2)$.

- β_1 = slope (1 unit increase in x corresponds to β_1 units change in y),
- β_0 = intercept (value at $x = 0$),
- σ = dispersion (stand. deviation) about line,
- ε_i = (vertical) error for i^{th} observation.

[3] i.i.d. = independent and identically distributed.

Simple Linear Regression – Analysis

Least squares estimation:

- idea: "best" line minimizes the sum of squared errors
$$\sum_i \varepsilon_i^2 = \sum_i (y_i - \beta_0 - \beta_1 x_i)^2,$$
- $\hat{\beta}_1$ and $\hat{\beta}_0$ unbiased and "optimal" under certain model assumptions,
- easy calculation formulae (simple regression only!),

$$\begin{aligned} \hat{\beta}_1 &= r s_y / s_x, \text{ where } r = \text{correlation betw. } x \text{ and } y \\ \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x}, \\ \hat{y} &= \hat{\beta}_0 + \hat{\beta}_1 x \quad \text{(estimated line).} \end{aligned}$$

Statistical inference about regression parameters:
the 4-step procedure, with $t(\text{DFE})$ as reference distribution.

ANOVA table for simple linear regression:

Source of variation	DF: Degrees of freedom	SS: Sum of squares	MS: Mean square	F
Reg. model	DFM$=1$	SSM	MSM$=$SSM$/1$	MSM/MSE
Error/Resid.	DFE$=n-2$	SSE$=\sum_i \hat{\varepsilon}_i^2$	MSE$=$SSE/DFE	
Total	DFT$=n-1$	SST		

- estimated error variance $= s^2 =$ MSE, as usual,
- F-test equivalent (same P) to t-test for $\beta_1 = 0$: $F = t^2$,
- $r^2 =$ SSM/SST, coefficient of determination, or proportion of variation explained (often denoted R^2).

4-Step Approach to Tests and CIs

- Data: $y_1, \ldots, y_n$,

1) Statistical model containing a (mean) parameter β,

2) Estimate $\hat{\beta}$ for β, based on $y_1, \ldots, y_n$.

3) Standard error $\text{SE}(\hat{\beta})$, either

   * estimated from the data, or
   * known value (rarely realistic in practice),

   Note: in normal models we often have

   $$\text{SE}(\hat{\beta}) = A\,\sigma \text{ (or, } \text{Var}(\hat{\mu}) = A^2\sigma^2),$$

   where σ is the standard deviation in the model, and A is a constant determined by the form of $\hat{\beta}$,

4) Reference distribution of $(\hat{\beta} - \beta)/\text{SE}(\hat{\beta})$,
   Note: in normal models with estimated $\text{SE}(\hat{\beta})$ the reference distribution is usually a $t(\text{DFE})$-distribution,

- Confidence interval $(1-\alpha)$ for β : $\hat{\beta} \pm t_{1-\alpha/2}\,\text{SE}(\hat{\beta})$,
- Test of H_0: $\beta = \beta^*$ against H_a: $\beta \neq \beta^*$, (β^* known value)

$$\text{test statistic} \qquad t = \frac{\hat{\beta} - \beta^*}{\text{SE}(\hat{\beta})},$$

$$P\text{-value} \qquad P = 2 \times \text{P}(t \geq |t_{\text{obs}}|),$$

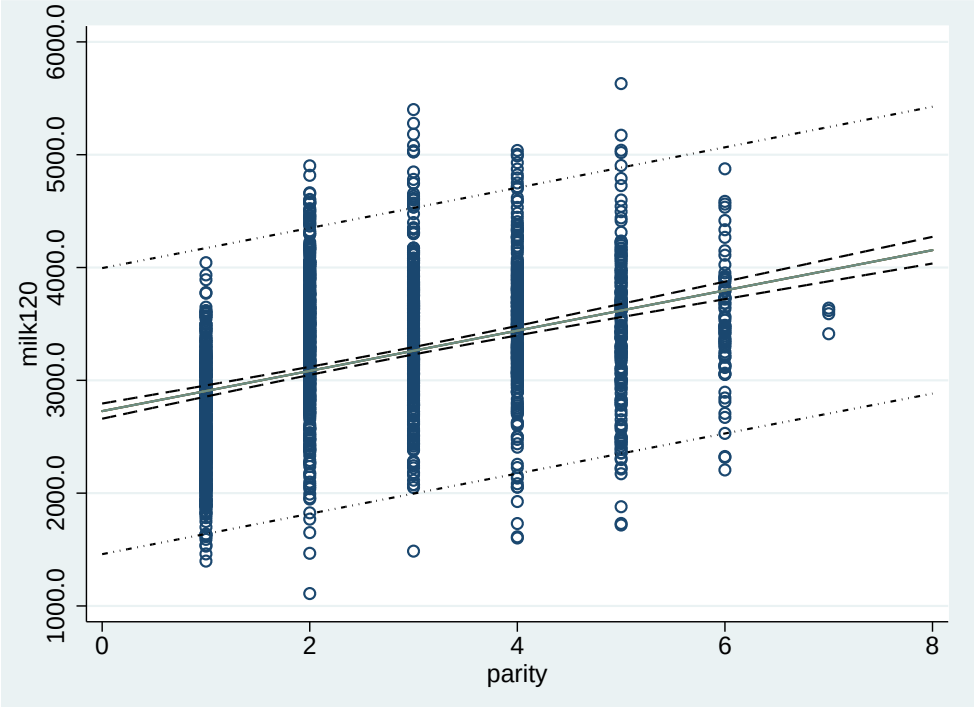
where $t \sim$ the reference distribution.

Prediction

Objective: give value and interval range (with confidence level $1-\alpha$) for a *new observation* with x-value x^*,

- predicted value $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x^*$ (estimated point on line),
- prediction interval (PI) wider than confidence interval[4] (CI) for point on the line, because it involves two types of variations:
  - $\mathrm{SE}(\hat{y}) \sim$ uncertainty in $\hat{\beta}$'s (which are not exactly equal to true β's),
  - $\sigma^2 \sim$ variation of the new observation itself,

  in a formula: prediction error $= \sqrt{(\mathrm{SE}(\hat{y}))^2 + \mathrm{MSE}}$,
  – use instead of $\mathrm{SE}(\hat{y})$ in 4-step approach to CIs.



[4] Stata terminology: prediction ∼ estimation, forecasting ∼ prediction.

Model Assumptions

Statistical assumptions:

- the linear relation: $\mathrm{E}y_i = \beta_0 + \beta_1 x_i$,[5]
- normal distribution of errors ε_i,[6]
- same variance (and standard deviation) of all errors (and observations[6]) − variance homogeneity or homoscedasticity, as opposed to heteroscedasticity,
- independence of errors (and of observations),
- x's considered fixed (measured without error, e.g. because controlled by experimenter);

  If x is an observed (response) variable,

  * the regression model is valid for *prediction* using observed x-values,
  * accounting for variability in x's requires a measurement error model (advanced).[7]

[5] Two types of linearity exist: in x and in the parameters (β_0, β_1); the former is relevant for model checking, the latter defines the class of "linear models". For example, the equation, $\mathrm{E}y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2$, defines a linear model but is not linear in x.

[6] If the errors (ε_i) are normally distributed with the same variance, then the same will be the case for the observations (y_i); however, this is of limited use for model checking because their means $(\mathrm{E}y_i)$ differ.

[7] (technical) It is true generally that the regression model estimates are biased towards the null for the true regression equation parameters, with a bias proportional to the variability in the x's.

Residuals

Overview: Residuals are estimates of the (unknown) errors and comprise the most useful tool for model checking, both for individual observations and overall; this is because the model assumptions are expressed through the errors (being i.i.d. and $\sim \mathrm{N}(0, \sigma^2)$).

- Raw/Simple residuals defined as:

  $\hat{\varepsilon}_i = y_i - \hat{y}_i = y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i)$ ("observed − expected"),

  properties (if model correct):
  normally distributed but *not* independent, with
  - mean 0, that is: $\mathrm{E}\,\hat{\varepsilon}_i = 0$,
  - computable variance, only constant in special cases,
- Standardised residuals:[8]

  $$r_i = \hat{\varepsilon}_i / \mathrm{SE}(\hat{\varepsilon}_i) \;\approx\; \mathrm{N}(0,1) \quad \text{(if model correct)},$$

  more powerful than raw residuals and with direct interpretation,
  - 95% of values expected between -2 and 2,
  - values outside ± 3.5 rare in moderately-sized dataset,
  - values outside ± 5 (almost) always suspect.

[8] The term "studentized residuals" is also used but this often leads to confusion because some sources further distinguish between two types of studentized residuals: internally studentized residuals (= standardised residuals), and externally studentized residuals (= deletion residuals, next slide).

Deletion Residuals

3-step calculation of deletion residual[9] d_i (for obs. i):

- compute fitted value $\tilde{y}_i$ for obs. i based on estimated model for all observations *excluding* observation i (idea: eliminate influence of obs. i on estimates),
- compute residual: $y_i - \tilde{y}_i$,
- standardise residual by dividing by its standard error (also based on model without obs. i).

Interpretation and use:

- for extreme obs., d_i usually somewhat more extreme than r_i (difference can be large, espec. in small datasets),
- can be used for outlier test[10]:
  - test statistic $= d_i$ (as provided by software),
  - reference distribution $= t(\text{DFE}-1)$, (in which one computes the tail probability),
  - unless strong "external suspicion" exists that obs. i is outlying[11], one should apply a Bonferroni correction for examining all observations as possible outliers:
    − change signif. level to $0.05/n$, or multiply P by n, where n = number of observations (including i).

[9] In Stata, unfortunately termed studentized residuals (see previous footnote).
[10] Null hypothesis H_0: obs. i is in agreement with model from rest of the data.
[11] The suspicion must not be based on the observed value y_i.

Assessment of Normality and Linearity

Normality is usually assessed by the standardised residuals:

- graphically: normal (quantile) plot/histogram for r_i's,
- descriptively: compute skewness and kurtosis for r_i's,
- formally using a statistical test for normality: should not be interpreted too rigidly, because
  - the residuals are not independent (one of the assumptions behind all normality tests)
  - the deviations from normality may be statistically significant (in a large data set) but of little importance for the statistical analysis.

Linearity or lack of fit (inadequacy of mean part of model) may also assessed by the standardised residuals:

- graphically: plot r_i's vs. x_i's and look for patterns deviating from horizontal line (maybe using lowess smoother),
- standard residual plot: plot r_i's vs. $\hat{y}_i$'s and look for any patterns beyond noise in a horizontal band which might be associated with missing predictors,[12]
- further graphical exploration: plot r_i's against any other variables of interest that might be related to the outcome (e.g., observation order).

[12] In simple linear regression, this plot contains the same information as the plot against the x_i's.

Assessment of Homoscedasticity

First thing to do:
plot standardised residuals against fitted values, and look for cone (fan) shape indicating residuals to be more variable at one end of the scale than the other.

Descriptive statistics: compute standard deviations of r_i's across groups defined in any "interesting" way.

Test for homoscedasticity? − no problem, many tests exist...,

- no overall best test (to my knowledge),
- the test may be more sensitive to model deviations than the least squares regression itself ("somewhat robust"),
- testing for homoscedasticity seems to be most popular in econometrics (and they spell it with a "k")...,
- some commonly used tests for ungrouped[13] ("regression") models (available in Stata):
  - Breusch-Pagan/Cook-Weisberg test (`hettest`),
    White's test (`imtest`),
- personal view: use these as "descriptive statistics" contributing to your information about the data/model, not as the ultimate truth (so don't use P-values too rigidly),
- truly robust methods exist:
  - robust standard errors (much later lecture),
  - robust regression − different statistical approach.

[13] For grouped ("ANOVA") models the most commonly used tests are: Levene's test (`sdtest`), Bartlett's test (`oneway`; very sensitive to model deviations).

Transformation in Regression Models

Potential aims of transformation:

1) obtain linear relation,

2) deal with unequal variances (depending on means),

3) deal with non-normal errors.

Aims may be conflicting (suggest different transformations)
$\Rightarrow$ transformation is "an art" (and a trial and error process).

Types of transformations:

- consider only transform of y (also possible: x, or both y and x),
- "standard" (variance-stabilising): log (natural or base 10) or square-root for right-skewed data, and $\arcsin(\sqrt{y})$ for proportion data,
- power transformations: $y \mapsto y^\lambda$ for some power λ.[14]

Statistical inference for transformation:

- estimation of power λ by Box-Cox method,
- associated CI (for λ) gives range of "plausible" values.

Results from transformed scale analysis *must!* be backtransformed to original scale:

- backtransformed means = medians in original data,
- for CIs: backtransform both endpoints,
- difficult to get means and SEs on original scale,
- backtransform β's only for log-transform; *never* backtransform SEs.

[14] Stata uses instead the Greek letter θ (theta) to represent the power: $y \mapsto y^\theta$.

Box-Cox Transformation

Applied view of Box-Cox transformation[15]:

- Box-Cox analysis (`boxcox` command in Stata) gives optimal transformation (among those considered...):
  - "optimal" $\sim$ make residuals fit as well as possible to a normal distribution with homogenenous variance,
  - transformation to make distribution of outcome close to normal is something else (*not recommended!*)[16],
- once optimal λ-value found, transform using simple formulae:

$$y \mapsto \begin{cases} y^{\lambda} & \text{for } \lambda > 0, \\ \ln(y) & \text{for } \lambda = 0, \\ -1/y^{|\lambda|} & \text{for } \lambda < 0, \end{cases}$$

- common practice to approximate optimal λ-value by a close "nice" value, e.g. 0.5, 0, -0.5 or -1 (to avoid too strange transformations),
- Box-Cox analysis requires all $y_i > 0$:
  - add a small value to meet requirement if only few $y_i = 0$ or $y_i < 0$,
  - Box-Cox type analysis possible (in S-Plus/R) also for transformations of the form: $y \mapsto \ln(y + \alpha)$. [16]
- redo model checks for transformed data! ("best" $\neq$ "good")

[15] Strictly speaking, it is the method of analysis rather than the transformation itself that carries the name of Box and Cox, after their 1964 paper in JRSSB.

[16] The Stata `ladder` and `lnskew0` commands should not be used for inference.

Box-Cox Transformation – Details

Box-Cox family of power transformations:

$$y \mapsto y^{(\lambda)} = \begin{cases} \frac{y^\lambda - 1}{\lambda}, & \text{for } \lambda \neq 0, \\ \ln(y), & \text{for } \lambda = 0, \end{cases}$$

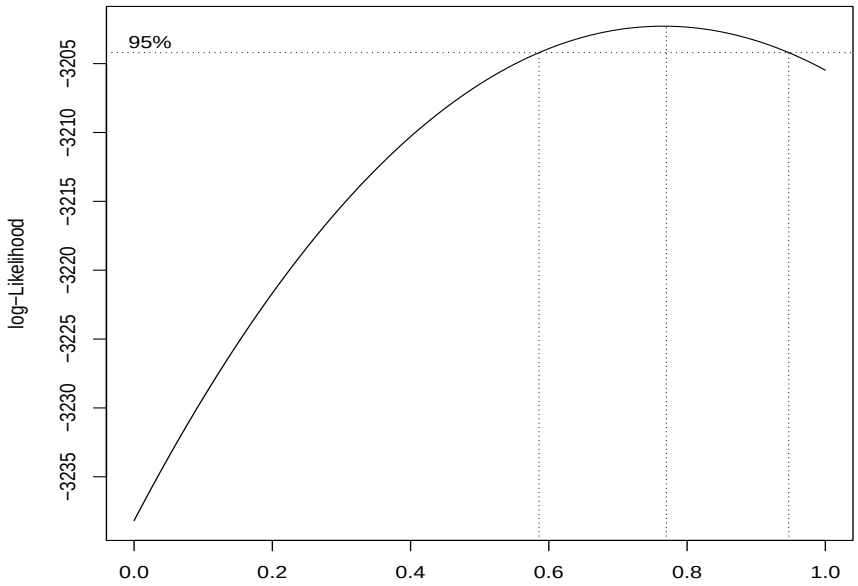
- the definition makes $y^{(\lambda)}$ continuous as a function of λ,
- very flexible class of transformations,
- maximum likelihood estimation of λ possible, by maximising the so-called (log) profile likelihood function, here denoted $\log L(\lambda)$,[17]
- manual maximisation most conveniently performed by plotting $\log L(\lambda)$ at a grid of λ-values,
- approximate 95% confidence interval for λ – several methods:
  - probably best CI is profile likelihood-ratio based, consisting of those λ-values where $\log L(\lambda)$ differs at most 1.82 from the optimal λ-value $\hat{\lambda}$,[18]
  - simpler CI uses estimate $\hat{\lambda}$ and its SE; probably ok in most cases (in particular for large sample size).

[17] Manual computation is possible but impractical; implementations exist in most statistical software: Stata (`boxcox` command), Minitab, SAS, S-Plus/R.

[18] The likelihood-ratio can also be used for a significance test comparing a specific λ-value to $\hat{\lambda}$: the `boxcox` command in Stata does this for $\lambda = -1, 0, 1$.

Box-Cox Analysis for `DAISY2`

Profile log-likelihood for regression of `milk120` on `parity`:



Conclusion: graph shows optimal λ-value around 0.75 and a 95% CI that excludes both 0.5 and 1.[19]

Comparison of model fits at different scales:

Scale of analysis	Original	Power	Square-root
Residual statistic	$\lambda = 1$	$\lambda = 0.75$	$\lambda = 0.5$
skewness	0.129	-0.023	-0.179
kurtosis (Stata)	3.090	3.071	3.138
normality (P^1)	0.065	0.614	0.012
homoscedast. (P^2)	0.007	0.069	0.362

[1] Shapiro-Wilk test (`swilk`); [2] BPCW test (`hettest`)

Conclusion: cannot achieve both perfect skewness and homoscedasticity: $\lambda = 0.75$ is a fair compromise, but model violations at $\lambda = 1$ and 0.5 hardly very serious for analysis.

[19] Estimation in Stata yields $\hat{\lambda} = 0.765$ with a 95% CI of $(0.585, 0.946)$.