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 14,
- notation of lecture(s) mainly follows GO, e.g. variables (e.g., x and y) are not capitalized.

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.

[1] Also General Linear Models (*not* Generalized!), e.g. Minitab & SAS software.

Dataset DAISY2

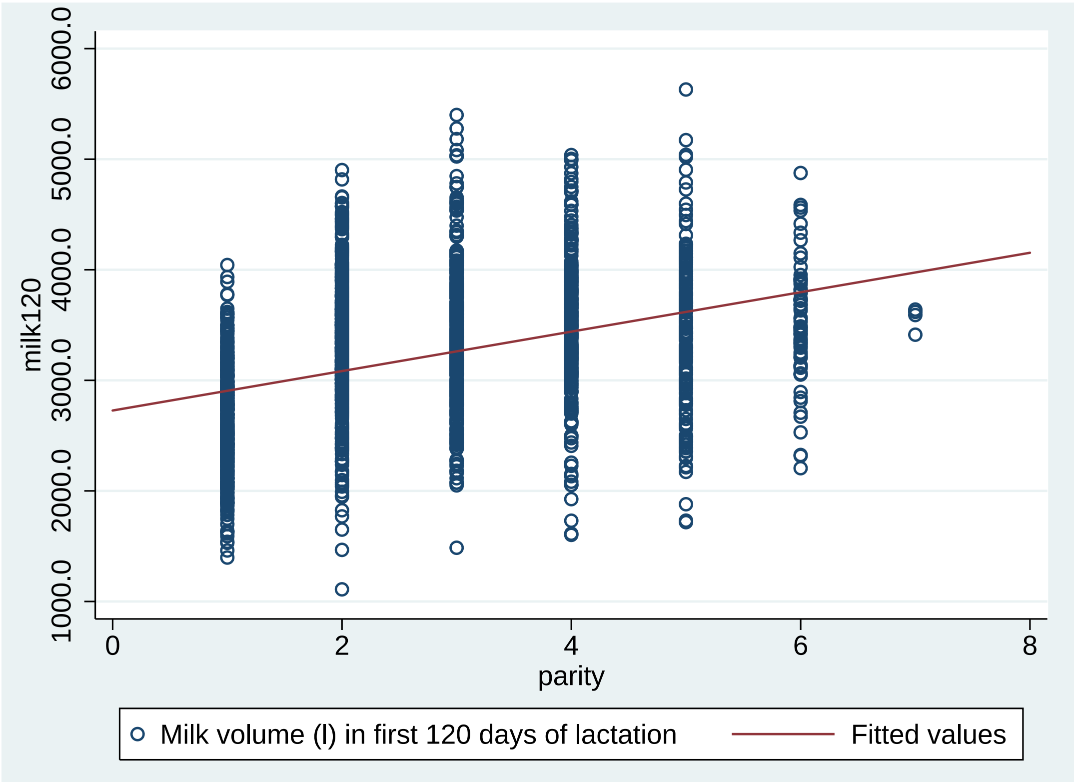
- VER2 dataset (from VER website),[2]
- real data ∼ single cohort study involving more than 8000 cows in 42 herds,
- contributed by John Morton, Australia,
- purpose of study: evaluate the effect of various diseases on milk yield and reproductive performance,
- focus here (and in entire VER Ch. 14) on 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 = stand. deviation ("dispersion") about the 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(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 $\mathrm{SE}(\hat\beta)$, either
   - ∗ estimated from the data, or
   - ∗ known value (rarely realistic in practice),

   Note: in normal models we often have
   $$\mathrm{SE}(\hat\beta) = A\,\sigma \text{ (or, } \mathrm{Var}(\hat\mu) = A^2\sigma^2),$$
   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 $(\hat\beta - \beta)/\mathrm{SE}(\hat\beta)$,
   Note: in normal models with estimated $\mathrm{SE}(\hat\beta)$ the reference distribution is usually a $t(\mathrm{DFE})$-distribution,

- Confidence interval $(1-\alpha)$ for β : $\hat\beta \pm t^* \,\mathrm{SE}(\hat\beta)$,[4]
- Test of H_0: $\beta = \beta^*$ against H_a: $\beta \neq \beta^*$, (β^* known value)

$$\text{test statistic} \qquad t = \frac{\hat\beta - \beta^*}{\mathrm{SE}(\hat\beta)},$$
$$P\text{-value} \qquad P = 2 \times \mathrm{P}(t \geq |t_{\mathrm{obs}}|),$$

where $t \sim$ the reference distribution.

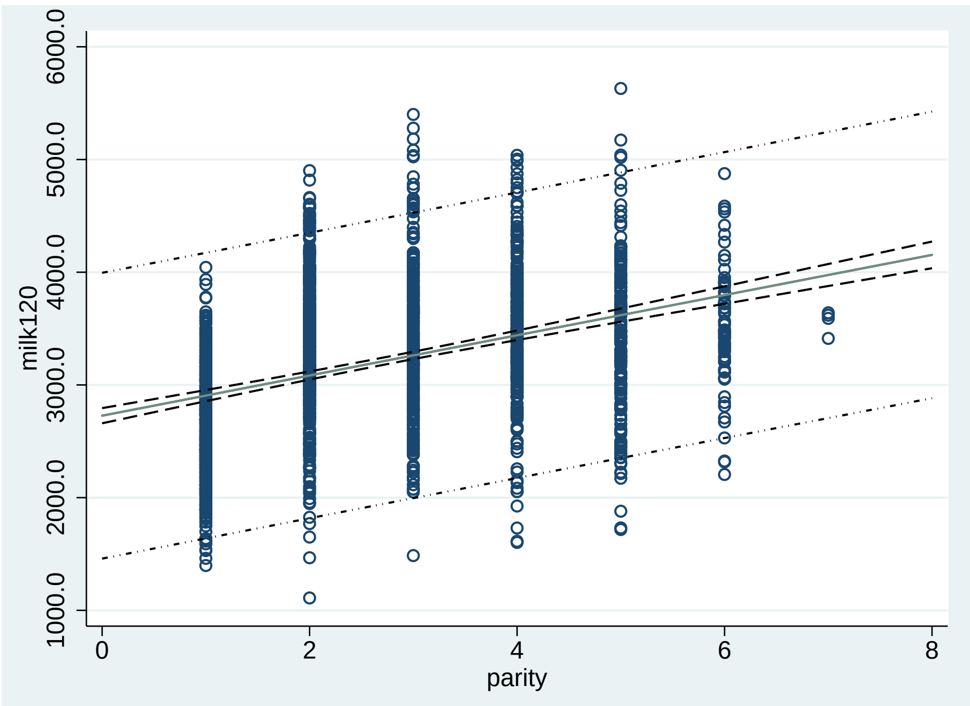
[4] In VHM 801 notation, $t^* = t_{1-\alpha/2} = t_{1-\alpha/2}(\mathrm{DFE})$, the $(1 - \frac{\alpha}{2})$-percentile of $t(\mathrm{DFE})$.

Prediction

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

- predicted value (point on line): $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x^*$,
- prediction interval (PI) wider than confidence interval[5] (CI) for point on the line, because it involves two types of variability:
  - $*$ $\text{SE}(\hat{y}) \sim$ uncertainty in $\hat{\beta}$'s (which are not exactly equal to true β's),
  - $*$ $\sigma^2 \sim$ variability of the new observation itself,

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



[5] Stata terminology: prediction $\sim$ estimation, forecasting $\sim$ prediction.

Model Assumptions

Statistical assumptions:

- the linear relation: $\mathrm{E}y_i = \beta_0 + \beta_1 x_i$,[6]
- normal distribution of errors [7] [8]: $\varepsilon_i \sim \mathrm{N}(0, \sigma^2)$,
- same variance (and standard deviation) of all errors (and observations[8]) − 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).[9]

[6] 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.

[7] Strictly speaking, normality for the *residuals* (next slide) is a consequence of the model, not an assumption.

[8] 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 no use for model checking because their means $(\mathrm{E}y_i)$ differ; *checking normality of* (y_i) *is pointless!!*

[9] (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:[10]

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

  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.

[10] 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[11] 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[12]:
  - 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[13], 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).

[11] In Stata, unfortunately termed studentized residuals (see previous footnote).
[12] Null hypothesis H_0: obs. i is in agreement with model from rest of the data.
[13] 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,[14]
- further graphical exploration: plot r_i's against any other variables of interest that might be related to the outcome (e.g., observation order).

[14] 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 (or predictors), and look for cone (fan) shape indicating residuals to be more variable at one end of the scale than the other.

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

Test for H_0: 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 ("which is 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[15] ("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.

[15] 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 variance (depending on the mean),

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),
- power transformations: $y \mapsto y^\lambda$ for some power λ, [16]
- "standard" variance-stabilising transformations:

Data type (y)	Mean	Variance	Transformation	Power[a]
measurement/conc.	$\mathrm{E}y = \mu$	$\mathrm{Var}y \propto \mu^2$	$\log(y)$ or $\ln(y)$	$\lambda = 0$
count	$\mathrm{E}y = \lambda$	$\mathrm{Var}y \propto \lambda$	$\sqrt{y}$	$\lambda = 0.5$
proportion	$\mathrm{E}y = p$	$\mathrm{Var}y \propto p(1-p)$	$\arcsin(\sqrt{y})$	n/a

[a] within Box-Cox family of power transform.: $y \mapsto \begin{cases} \frac{y^\lambda - 1}{\lambda} & \text{for } \lambda \neq 0, \\ \ln(y) & \text{for } \lambda = 0. \end{cases}$

Statistical inference for transformation:

- estimation[17] of transformation power λ within Box-Cox family,
- associated CI (for λ) gives range of "plausible" values and can be used in significance testing for specific λ-values (e.g., $H_0 : \lambda = 1$).[18]

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

[17] (technical) Maximum likelihood estimation, by maximising the so-called (log) profile likelihood function, either by an automatic software routine (Stata, Minitab) or by manual maximisation across a grid of λ-values (S-Plus/R).

[18] (technical) Both likelihood- and Wald-methods usually give sensible results.

Box-Cox Transformation

Applied view of Box-Cox transformation[19]:

- Box-Cox analysis (`boxcox` command in Stata) gives optimal transformation (among those considered…):
  - ∗ "optimal" ∼ 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!*)[20],
- once optimal λ-value found, transform using simple formulae:

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

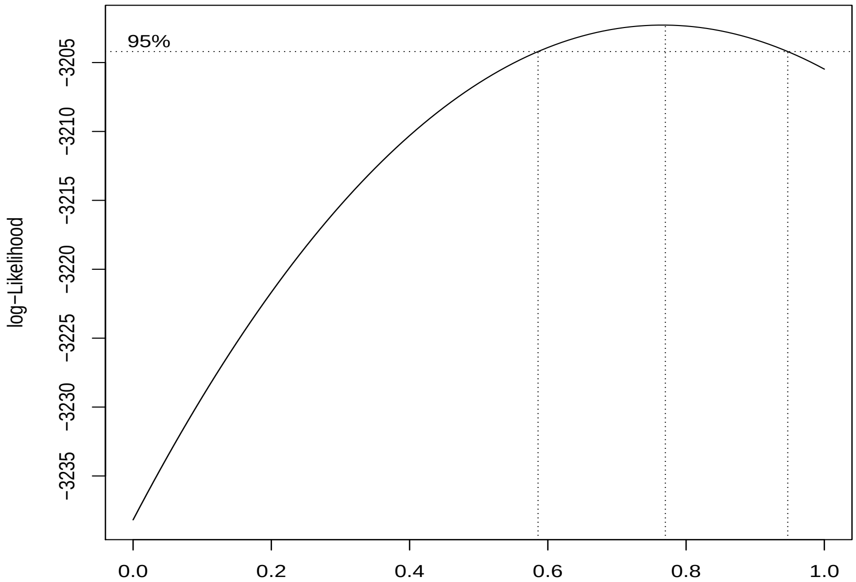
- common practice to approximate optimal λ-value by a close "nice" value, e.g. 0.5, 0, -0.5 or -1 (to avoid too strange transformations),
- Box-Cox analysis requires all $y_i > 0$:
  - ∗ add a small value to meet requirement if only few $y_i = 0$ or $y_i < 0$,
  - ∗ Box-Cox type analysis possible (in S-Plus/R) also for transformations of the form: $y \mapsto \ln(y + \alpha)$. [20]
- redo model checks for transformed data! ("best" ≠ "good")

[19] 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.

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

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.[21]

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.

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

Backtransformation in Regression Models

Main message: Results from transformed scale analysis must! (nearly always) be backtransformed to original scale.

General rules (valid for any monotonic transformation):

- backtransformed means $\sim$ medians (*not* means) at original scale,
- CIs can be backtransformed by backtransforming both endpoints,
- difficult to get means and SEs at original scale,[22]
- backtransform regression parameters (β's) only for log-transform (below); *never* backtransform their SEs.

Special procedures for log-transformation[23]; consider the model

$$\begin{aligned} \ln(y_i) &= \beta_0 + \beta_1 x_i + \varepsilon_i, \qquad \text{or} \\ y_i &= \mathrm{e}^{\beta_0} \cdot \mathrm{e}^{\beta_1 x_i} \cdot \mathrm{e}^{\varepsilon_i}. \end{aligned}$$

Disregarding the error terms (involving ε_i), we get the interpretations:

* $\mathrm{e}^{\beta_0} \sim$ median value at original scale for $x = 0$,
* $\mathrm{e}^{\beta_1} \sim$ *multiplicative* effect of a 1-unit increase in x;
  example: if $\beta_1 = 0.4$, then $\mathrm{e}^{\beta_1} \approx 1.49 \sim$ multiplication by 1.49, or a relative increase by 49%,
* if the x's are also on logarithmic scale (say $x = \ln(z)$), then a 1-unit increase in $x \sim$ an increase in z by a factor of $\mathrm{e}^1 = 2.72$; instead, we may consider a change in x by $\ln(2) = 0.693$, corresponding to an increase in z by a factor of 2 (i.e., a doubling);
  example: if $\beta_1 = 0.4$, then $\mathrm{e}^{\beta_1 \cdot \ln(2)} \approx 1.32 \sim$ multiplication by 1.32, or a relative increase by 32%, for a doubling in z.

[22] Simulation approaches, beyond the scope of the course, can be used.
[23] Described here for natural log, but works also for other logarithms by replacing the exponential function by the appropriate inverse logarithmic function.