An introduction to statistical analysis

Overheads

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Topic: Motivation

Why is statistics important?

It is part of the quantitative approach to knowledge:

"In physical science the first essential step in the direction of learning any subject is to find principles of numerical reckoning and practicable methods for measuring some quality connected with it.

"I often say that when you can measure what you are speaking about, and express it in numbers, you know something about it;

- "...but when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind;
- "... it may be the beginning of knowledge, but you have scarcely in your thoughts advanced to the state of Science, whatever the matter may be."
- Lord Kelvin (William Thomson), Popular Lectures and Addresses 1:73



A simple definition

Statistics: "The determination of the probable from the possible"

- Davis, Statistics and data analysis in geology, p. 6
- ... which implies the rigorous definition and then quantification of "probable".
- Probable causes of past events or observations
- Probable occurrence of future events or observations

This is a definition of **inferential** statistics:

Observations ⇒ Inferences



What is "statistics"?

Two common use of the word:

- 1. **Descriptive** statistics: numerical summaries of **samples**;
 - (what was observed)
- 2. Inferential statistics: from samples to populations.
 - (what could have been or will be observed)

Example:

Descriptive "The adjustments of 14 GPS control points for this orthorectification ranged from 3.63 to 8.36 m with an arithmetic mean of 5.145"

Inferential "The mean adjustment for any set of GPS points used for orthorectification is no less than 4.3 and no more than 6.1 m; this statement has a 5% probability of being wrong."



Why use statistical analysis?

- 1. Descriptive: we want to summarize some data in a shorter form
- 2. Inferential: We are trying to understand some process and possible predict based on this understanding
 - So we need model it, i.e. make a conceptual or mathematical representation, from which we infer the process.
 - But how do we know if the model is "correct"?
 - Are we imagining relations where there are none?
 - * Are there true relations we haven't found?
 - Statistical analysis gives us a way to quantify the confidence we can have in our inferences.



Topic: Introduction

- 1. Outline of statistical analysis
- 2. Types of variables
- 3. Statistical inference
- 4. Data analysis strategy
- 5. Univariate analysis
- 6. Bivariate analysis; correlation; linear regression
- 7. Analysis of variance
- 8. Non-parametric methods



Reference web pages

- Electronic Statistics Textbook: [StatSoft]
 http://www.statsoftinc.com/textbook/stathome.html
- NIST/SEMATECH e-Handbook of Statistical Methods: http://www.itl.nist.gov/div898/handbook/
- HyperStat Online Textbook: http://davidmlane.com/hyperstat/
- The R environment for statistical computing and graphics: http://www.r-project.org/
- StatLib: "a system for distributing statistical software, datasets, and information" http://lib.stat.cmu.edu/



Texts

There are hundreds of texts at every level and for every application. Here are a few I have found useful.

Elementary:

- Bulmer, M.G., 1979. Principles of statistics. Dover Publications, New York.
- Dalgaard, P., 2002. Introductory Statistics with R. Springer-Verlag.

Advanced:

- Venables, W.N. and Ripley, B.D., 2002. Modern applied statistics with S. Springer-Verlag.
- Fox, J., 1997. Applied regression, linear models, and related methods. Sage, Newbury Park.



Applications:

- Davis, J.C., 2002. Statistics and data analysis in geology. John Wiley & Sons, New York.
 - * Website:

http://www.kgs.ku.edu/Mathgeo/Books/Stat/index.html

 Webster, R. and Oliver, M.A., 1990. Statistical methods in soil and land resource survey. Oxford University Press, Oxford.



Topic: Outline of statistical analysis

- What is statistical analysis?
- Populations, samples, outliers
- Steps in statistical analysis



What is "statistical analysis"?

This term refers to a wide range of techniques to...

- 1. (Describe)
- 2. Explore
- 3. Understand
- 4. Prove
- 5. Predict
- ... based on **sample datasets** collected from **populations**, using some **sampling strategy**.



Why use statistical analysis?

- 1. We want to summarize some data in a shorter form
- 2. We are trying to **understand** some process and possible **predict** based on this understanding
 - So we need model it, i.e. make a conceptual or mathematical representation, from which we infer the process.
 - But how do we know if the model is "correct"?
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 - Statistical analysis gives us a way to quantify the confidence we can have in our inferences.



Populations and samples

- Population: a set of elements (individuals)
 - * Finite vs. "infinite"
- Sample: a subset of elements taken from a population
 - * Representative vs. biased
- We make inferences about a population from a sample taken from it.
- In some situations we can examine the entire population; then there is no inference from a sample. Example: all pixels in an image.



Step 1: Outliers

Three uses of this word:

- An observation that is some defined distance away from the sample mean (an empirical outlier;
- 2. An extreme member of a population;
- 3. An observation in the **sample** that is *not* part of the population of interest.

Example: In a set of soil samples, one has an order of magnitude greater level of heavy metals (Cd, Pb, Cu etc.) than all the others.

- 1. The sample is an empirical outlier because it is more than 1.5 times the inter-quartile range from the 3rd quartile;
- 2. This is an extreme value but is included in our analysis of soil contamination;
- 3. This sample comes from an industrial site and is not important for our target population of agricultural soils.



Step 1: Explore & Describe

- Questions
 - * What is the **nature of the dataset** (lineage, variables ...)?
 - * What is the relation of the dataset to the underlying population(s)?
- Techniques
 - Graphical (visualisation): humans are usually good at picking out patterns
 - Numerical: summaries of outstanding features (descriptive statistics)
 - * These may suggest hypotheses and appropriate analytical techniques



Step 2: Understand

- If there is an underlying process of which the sampled data are a representative sample . . .
- ... then the data allow us to infer the nature of the process
- Example: the distribution of heavy metals in soil is the result of:
 - * Parent material
 - * Pollutants transported by wind, water, or humans
 - * Transformations in the soil since deposition
 - Movement of materials within and through the soil
 - *
- Summarize the understanding with a model



What is a statistical model?

- A mathematical representation of a process or its outcome . . .
- ... with a computable level of uncertainty
- ...according to assumptions (more or less plausible or proveable)

This is an example of an **empirical** model. It may **imply** the underlying process, but need not. It might be useful for **prediction**, even if it's a "black box".

Assumptions: not part of the model, but must be true for the model to be correct.

(Note: A process model explicitly represents the underlying process and tries to simulate it.)



Step 3: "Prove"

A further step is to "prove", in some sense, a statement about nature.

E.g. "Soil pollution in this area is caused by river flooding; pollutants originate upstream in industrial areas."

- The model must be plausible → evidence of causation
- With what confidence can we state that our understanding (model) is correct?
- Nothing can be proved absolutely; statistics allows us to accumulate evidence
- We can determine sampling strategies to achieve a given confidence level
- Underlying assumptions may not be proveable, only plausible



Step 4: Predict

- The model can be applied to unsampled entities in the underlying population
 - Interpolation: within the range of the original sample
 - Extrapolation: outside this range
- The model can be applied to future events; this assumes that future conditions (the context in which the events will take place) is the same as past conditions (c.f. "uniformitarianism" of Hutton and Playfair)
- A *geo*-statistical model can be applied to **unsampled locations**; this assumes that the process at these locations is the same as at the sample locations.

Key point: we must **assume** that the **sample** on which the model is based is **representative** of the **population** in which the predictions are made. We argue for this with **meta-statistical analysis** (outside of statistics itself).



Topic: Types of variables

In order of information content (least to most):

- 1. Nominal
- 2. Ordinal
- 3. Interval
- 4. Ratio



Nominal variables

- Values are from a set of classes with no natural ordering
- Example: Land uses (agriculture, forestry, residential . . .)
- Can determine equality, but not rank
- Meaningful sample statistics: mode (class with most observations); frequency distribution (how many observations in each class)
- Numbers may be used to label the classes but these are arbitrary and have no numeric meaning (the "first" class could just as well be the "third"); ordering is by convenience (e.g. alphabetic)
- R: "unordered factors"



Ordinal variables

- Values are from a set of naturally ordered classes with no meaningful units of measurement
- Example: Soil structural grade (0 = structureless, 1 = very weak, 2 = weak, 3 = medium, 4 = strong, 5= very strong)
- N.b. This ordering is an intrinsic part of the class definition
- Can determine rank (greater, less than)
- Meaningful sample statistics: mode; frequency distribution
- Numbers may be used to label the classes; their order is meaningful, but not the intervals between adjacent classes are not defined (e.g. the interval from 1 to 2 vs. that from 2 to 3)
- R: "ordered factors"



Interval variables

- Values are measured on a continuous scale with well-defined units of measurement but no natural origin of the scale, i.e. the zero is arbitrary, so that differences are meaningful but not ratios
- Example: Temperature in °C.
- "It is twice as warm yesterday as today" is meaningless, even though "Today it is 20°C and yesterday it was 10°C" may be true.
 - (To see this, try the same statement with Farenheit temperatures)
- Meaningful statistics: quantiles, mean, variance



Ratio variables

- Values are measured on a continuous scale with well-defined units of measurement and a natural origin of the scale, i.e. the zero is meaningful
- Examples: Temperature in °K; concentration of a chemical in solution
- "There is twice a much heat in this system as that" is meaningful, if one system is at $300^{\circ} \mathrm{K}$ and the other at $150^{\circ} \mathrm{K}$
- Meaningful statistics: quantiles, mean, variance; also the coefficient of variation. (Recall: CV = SD / Mean; this is a ratio).



Continuous vs. discrete

Interval and ratio variables can be either:

Discrete Taking one of a limited set of discrete values, e.g. integers

Continuous Can take any value (limited by precision) in a defined range

 Not "continuous" in the strict mathematical sense (because the computer can only represent rational numbers)



Topic: Statistical Inference

One of the main uses of statistics is to infer from a sample to a population, e.g.

- the "true" value of some parameter of interest (e.g. mean)
- the degree of support for or against a hypothesis

This is a contentious subject; here we use simple "frequentist" notions.



Statistical inference

- Using the sample to infer facts about the underlying population of which (we hope) it is representative
- Example: true value of a population mean, estimated from sample mean and its standard error
 - confidence intervals: having a known probability of containing the true value
 - * For a sample from a normally-distributed variate, 95% probability ($\alpha = 0.05$):

$$\overline{x} - 1.96 \cdot s_{\overline{X}} \le \mu \le \overline{x} + 1.96 \cdot s_{\overline{X}}$$

The standard error is estimated from the sample variance:

$$s_{\overline{X}} = \sqrt{s_X^2/n}$$



Inference from small samples

- Probabilities are referred to the t (Student's) distribution, rather than the z (Normal) distribution
- This corrects for the fact that we are estimating both the mean and variance from the same sample, and the variance is difficult to estimate from small samples

$$(\overline{x} - t_{\alpha=0.05,n-1} \cdot s_{\overline{X}}) \leq \mu \leq (\overline{x} + t_{\alpha=0.05,n-1} \cdot s_{\overline{X}})$$

- t from tables; $t \rightarrow z$ as $n \rightarrow \infty$
- $t_{\alpha=0.05,10}=2.228$, $t_{\alpha=0.05,30}=2.042$, $t_{\alpha=0.05,120}=1.980$



What does this really mean?

- "There is only a 1 in 20 chance that the true value of the population mean is outside this interval"
 - * If the sample is representative of the population
 - * If the distribution of values in the sample satisfies the requirements of the inferential method
- "If we repeat the same sampling strategy again (collecting a new sample), there is only a 1 in 20 chance that the confidence interval constructed from that sample will not contain the mean value from this first sample"
- This does not mean that 95% of the sample or population is within this interval!



The null and alternate hypotheses

- Null hypothesis H_0 : Accepted until proved otherwise ("innocent until proven guilty")
- Alternate hypothesis H₁: Something we'd like to prove, but we want to be fairly sure
- In the absence of prior information, the null hypothesis is that there is no relation
 - Classic example: a new crop variety does not (null) have a higher yield than the current variety (note one-tailed hypothesis in this case)
- But may use prior information for an 'informative' null hypothesis



Significance levels and types of error

- α is the risk of a **false positive** (rejecting the null hypothesis when it is in fact true), the **Type I** error
 - * "The probability of convicting an innocent person" (null hypothesis: innocent until proven guilty)
- β is the risk of a **false negative** (accepting the null hypothesis when it is in fact false), the **Type II** error.
 - "The probability of freeing a guilty person"
- α set by analyst, β depends on the form of the test



Selecting a confidence level

These must be balanced depending on the **consequences** of making each kind of error. For example:

- The cost of introducing a new crop variety if it's not really better (Type I), vs.
- The lost income by not using the truly better variety (Type II)
- The British legal system is heavily weighted towards low Type I errors (i.e. keep innocent people out of prison)
- The Napoleonic system accepts more Type I error in order to lower Type II error (i.e. keep criminals off the street)

(Or, the British and Napoleonic systems may have opposite null hypotheses.)



Topic: Data anlysis strategy

- 1. Posing the research questions
- 2. Examining data items and their support
- 3. Exploratory non-spatial data analysis
- 4. Non-spatial modelling
- 5. Exploratory spatial data analysis
- 6. Spatial modelling
- 7. Prediction
- 8. Answering the research questions



Research questions

 What research questions are supposed to be answered with the help of these data?



Data items and their support

- How were the data collected (sampling plan)?
- What are the variables and what do they represent?
- What are the units of measure?
- What kind of variables are these (nominal, ordinal, interval, or ratio)?
- Which data items could be used to stratify the population?
- Which data items are intended as response variables, and which as predictors?



Non-spatial modelling

- Univariate descriptions: normality tests, summary statistics
- Transformations as necessary and justified
- Bivariate relations between variables (correlation)
- Multivariate relations between variables
- Analysis of Variance (ANOVA) on predictive factors (confirms subpopulations)



Exploratory spatial data analysis

If the data were collected at known points in geographic space, we should visualise them in that space.

- Postplots: where are which values?
- Geographic postplots: with images, landuse maps etc. as background: do there appear to be any explanation for the distribution of values?
- Spatial structure: range, direction, strength . . .
- Is there anisotropy? In what direction(s)?
- Populations: one or many?



Spatial modelling

If the data were collected at known points in geographic space, it may be possible to model this.

- Model the spatial structure
 - Local models (spatial dependence)
 - Global models (geographic trends, feature space predictors)
 - * Mixed models



Prediction

- Values at points or blocks
- Summary values (e.g. regional averages)
- Uncertainty of predictions



Answer the research questions

- How do the data answer the research question?
- Are more data needed? If so, how many and where?



Topic: The Meuse soil pollution data set

This will be used as a **running example** for the following lectures.

It is an example of an "environmental" dataset which can be used to answer a variety of practical and theoretical research question.



Source

Rikken, M.G.J. & Van Rijn, R.P.G., 1993.

Soil pollution with heavy metals – An inquiry into spatial variation, cost of mapping and the risk evaluation of copper, cadmium, lead and zinc in the floodplains of the Meuse west of Stein, the Netherlands.

Doctoraalveldwerkverslag, Dept. of Physical Geography, Utrecht University

This data set is also used as an example in gstat and in the GIS text of Burrough & McDonnell.



Variables

155 samples taken on a support of 10x10 m from the top 0-20 cm of alluvial soils in a 5x2 km part the floodplain of the Maas (Meuse) near Stein (NL).

id	point number
x, y	coordinates E and N in Dutch national grid coordinates, in meters
cadmium	concentration in the soil, in mg kg ⁻¹
copper	concentration in the soil, in mg kg ⁻¹
lead	concentration in the soil, in mg kg ⁻¹
zinc	concentration in the soil, in mg kg ⁻¹
elev	elevation above local reference level, in meters
om	organic matter loss on ignition, in percent
ffreq	flood frequency class, 1: annual, 2: 2-5 years, 3: every 5 years
soil	soil class, coded
lime	has the land here been limed? $0 \text{ or } 1 = F \text{ or } T$
landuse	land use, coded
dist.m	distance from main River Maas channel, in meters



Accessing the Meuse data set

In R:

```
> library(gstat)
> data(meuse)
> str(meuse)
```

To import in other programs: comma-separated value (CSV) file meuse.csv.

```
"x", "y", "cadmium", "copper", "lead", "zinc", "elev", "dist", "om", "ffreq", "soil", "lime", "landuse", 181072, 333611, 11.7, 85, 299, 1022, 7.909, 0.00135803, 13.6, "1", "1", "1", "Ah", 50 181025, 333558, 8.6, 81, 277, 1141, 6.983, 0.01222430, 14.0, "1", "1", "1", "Ah", 30 ...
```



Topic: Probability

- 1. probability
- 2. discrete and continuous probability distributions
- 3. normality, transformations



Probability

- A very controversial topic, deep relation to philosophy;
- Two major concepts: Bayesian and Frequentist;
- The second can model the first, but not vice-versa;
- Most elementary statistics courses and computer programs take the frequentist point of view.

The probability of an event is:

Bayesian degree of rational belief that the event will occur, from 0 (impossible) to 1 (certain)

Frequentist the proportion of time the event would occur, should the "experiment" that gives rise to the event be repeated a large number of times



Frequentist concept of probability

- Intutively-appealing if an experiment can easily be repeated or another sample easily be taken, under the same conditions.
 - Often the case in earth sciences: if we have 100 soil samples we could (if budget allows) take 100 more; effectively there are an infinite number of possible samples
- Not so helpful with rare events
 - What is the frequentist "probability" of a major earthquake in the next year?
 - * This is why Bayesian methods (e.g. weights of evidence) are often used in risk assessment.



Probability distributions

- A complete account of the probability of each possible outcome . . .
- assuming some underlying process
- n.b. the sum of the probabilities of all events is by definition 1 (it's certain that something will happen!)

Examples:

- Number of radioactive decays in a given time period: Poisson
 - * assuming exponential decay with constant half-life, independent events.
- Number of successes in a given number of binary ("Bernoulli") trials (e.g. finding water within a fixed depth): Binomial
 - * assuming constant probability of success, independent trials



Probability vs. reality

- Frequentist probability refers to an idealized world with perfect mathematical properties;
- It is useful if we can argue that the assumptions are met;
- This is a meta-statistical argument.

Example: to describe a well-drilling programme with the binomial distribution, we must argue that:

- 1. An attempt can be unambiguously classified as a success or failure;
- 2. Every attempt to drill a well is independent;
- 3. Every attempt to drill a well has the same (possibly unknown) probability of success.

Only then can we model the campaign with a binomial distribution.



The Binomial distribution

This is a **discrete** probability distribution:

 Probability Density Function (PDF) of x successes in n trials, each with probability p of success:

$$f(x) = \binom{n}{x} p^x (1-p)^{n-x}$$

where

$$\binom{n}{x} \equiv \frac{n!}{x!(n-x)!}$$

is the **binomial coefficient**, i.e. the number of different ways of selecting x distinct items out of n total items.

Mean and variance:

$$\mu = np; \sigma^2 = np(1-p)$$

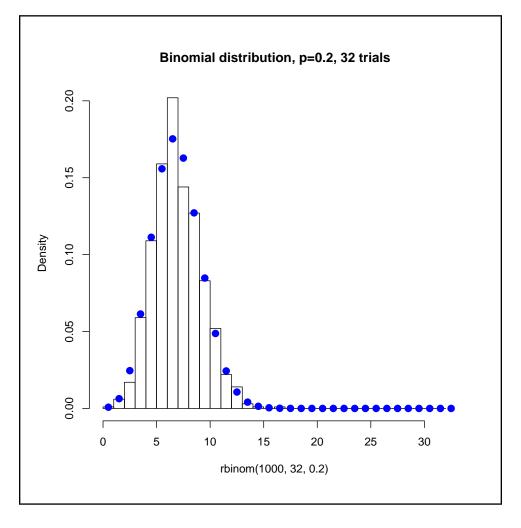


Example computation in R

```
> # number of distinct ways of selecting 2 from 16
> (f2 <- factorial(16)/(factorial(2)*factorial(16-2)))</pre>
[1] 120
> # direct computation of a single binomial density
> # for prob(success) = 0.2
> p <- 0.2; n <- 16; x <- 2
> f2 * p^x * (1-p)^(n-x)
[1] 0.21111
> # probability of 0..16 productive wells if prob(success) = 0.2
> round(dbinom(0:16, 16, 0.2),3)
 [1] 0.028 0.113 0.211 0.246 0.200 0.120 0.055 0.020
[9] 0.006 0.001 0.000 0.000 0.000 0.000 0.000
[17] 0.000
> # simulate 20 drilling campaigns of 16 wells, prob(success) = 0.2
> trials <- rbinom(20, 16, .2)
> summary(trials)
  Min. 1st Qu. Median Mean 3rd Qu.
                                         Max.
   1.00
          2.75
                  3.00 3.45
                                 4.00
                                          8.00
> # compare with theoretical mean and variance
> (mu <- n * p)
[1] 3.2
> (var <- n * p * (1-p)); var(trials)
[1] 2.56
[1] 2.2605
> sort(trials)
 [1] 1 2 2 2 2 3 3 3 3 3 3 4 4 4 4 4 4 5 5 8
```



Graph of an empirical vs. theoretical binomial distribution



```
> hist(rbinom(1000, 32, .2), breaks=(0:32), right=F, freq=F,
+ main="Binomial distribution, p=0.2, 32 trials")
> points(cbind((0:32)+0.5,dbinom(0:32, 32, 0.2)), col="blue",
+ pch=20, cex=2)
```



The Normal (Gaussian) probability distribution

This is a **continuous** probability distribution.

- Arises naturally in many processes: a variables that can be modelled as a sum of many small contributions, each with the same distribution of errors (central limit theorem)
- Easy mathematical manipulation
- Fits many observed distributions of errors or random effects
- Some statistical procedures require that a variable be at least approximately normally distributed
- Note: even if a variable itself is not normally distributed, its mean may be, since the deviations from the mean may be the "sum of many small errors".



Mathematical form of the Normal distribution

• Probability Density Function (pdf) with mean μ , standard deviation σ

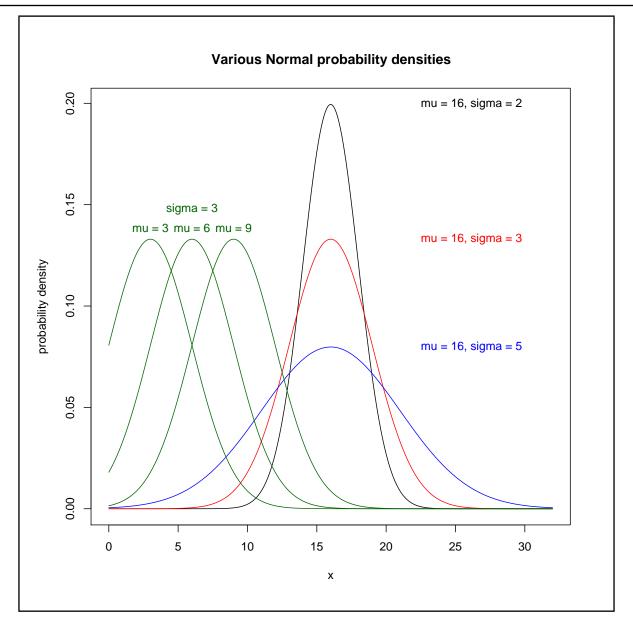
$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-(x-\mu)^2/2\sigma^2}$$
 $\int_{x=-\infty}^{\infty} f(x) = 1$

Cumulative Density Function (cdf)

$$F(z) = \int_{x = -\infty}^{z} f(x)$$

```
> # 8 normal variates with mean 1.6, var .2
> rnorm(8, 1.6, .2)
[1] 1.771682 1.910130 1.518092 1.712963 1.365242 1.837332 1.777395 1.749878
> # z-values for some common probabilities
> qnorm(seq(0.80,0.95, by=.05),1.6,.2)
[1] 1.768324 1.807287 1.856310 1.928971
```





- > range <- seq(0,32, by=.1)
- > plot(range, dnorm(range, 16, 2), type="l") # etc.



Standardization

- All normally-distributed variates can be directly compared by **standardization**: subtract μ , divide by σ
- Standardized normal: all variables have the same scale and deviation:

$$\mu = 0, \sigma = 1$$

$$f(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$$

```
> sdze < -function(x) \{ (x-mean(x))/sd(x) \}
```

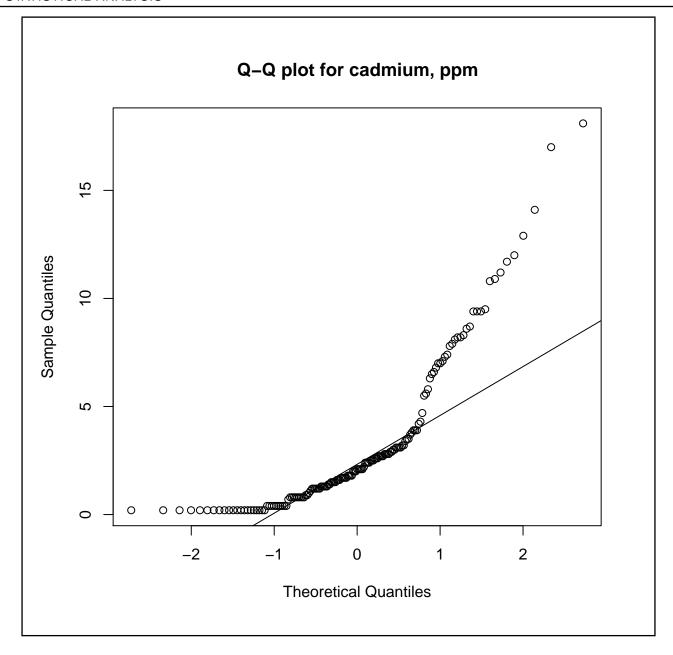


Evaluating Normality

- Graphical
 - * Histograms
 - Quantile-Quantile plots (normal probability plots)
- Numerical
 - Various tests including Kolmogorov-Smirnov, Anderson-Darling, Shapiro-Wilk
 - * These all work by compare the observed distribution with the theoretical normal distribution having parameters estimated from the observed, and computing the probability that the observed is a realisation of the theoretical

```
> qqnorm(cadmium); qqline(cadmium)
> shapiro.test(cadmium)
Shapiro-Wilk normality test
W = 0.7856, p-value = 8.601e-14
```



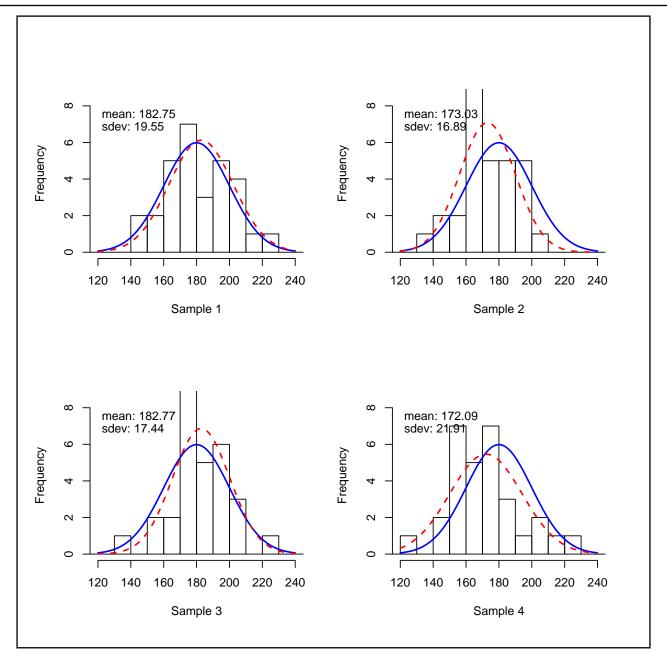




Variability of small samples from a normal distribution

Can we infer that the population is normal from a small sample?







Transforming to Normality: Based on what criteria?

These are listed in order of preference:

- 1. A priori understanding of the process
 - e.g. lognormal arises if contributing variables multiply, rather than add
- 2. EDA: visual impression of what should be done
- 3. Results: transformed variable appears and tests normal



Transforming to Normality: Which transformation?

- $x' = \ln(x+a)$: **logarithmic**; removes positive skew note: must add a small adjustment to zeroes
- $x' = \sqrt{x}$: square root: removes moderate skew
- $x' = \sin^{-1} x$: arcsine: for proportions $x \in [0...1]$ spreads the distribution near the tails
- $x' = \ln[x/(1-x)]$: **logit** (logistic) for proportions $x \in [0...1]$ note: must add a small adjustment to zeroes

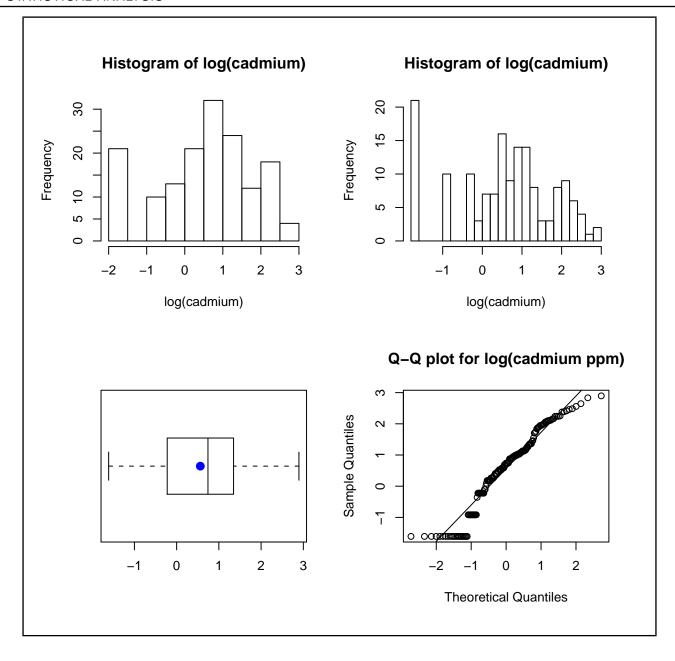


Example: log transform of a variable with positive skew

```
> summary(log(cadmium))
  Min. 1st Ou. Median
                           Mean 3rd Ou.
                                           Max.
-1.6090 -0.2231 0.7419 0.5611 1.3480 2.8960
> stem(logcad)
> hist(log(cadmium))
> hist(log(cadmium), n=20)
> plot(ecdf(log(cadmium)))
> boxplot(log(cadmium), horizontal=T)
> points(mean(log(cadmium)),1, pch=20, cex=2, col="blue")
> gqnorm(log(cadmium), main="Q-Q plot for log(cadmium ppm)")
> qqline(log(cadmium))
> shapiro.test(log(cadmium))
Shapiro-Wilk normality test
W = 0.9462, p-value = 1.18e-05
```

This is still not normal, but much more symmetric







Topic: Non-spatial univariate Exploratory Data Analysis (EDA)

- 1. exploratory data analysis
- 2. descriptive statistics



Exploratory Data Analysis (EDA)

- Statistical analysis should lead to understanding, not confusion . . .
- ...so it makes sense to examine and visualise the data with a critical eye to see:
 - 1. Patterns; outstanding features
 - 2. unusual data items (not fitting a pattern); blunders? from a different population?
 - 3. Promising analyses
- Reconaissance before the battle
- Draw obvious conclusions with a minimum of analysis



Graphical Univariate EDA

- Boxplot, stem-and-leaf plot, histogram, empirical CDF
- Questions
 - One population or several?
 - * Outliers?
 - Centered or skewed (mean vs. median)?
 - * "Heavy" or "light" tails (kurtosis)?

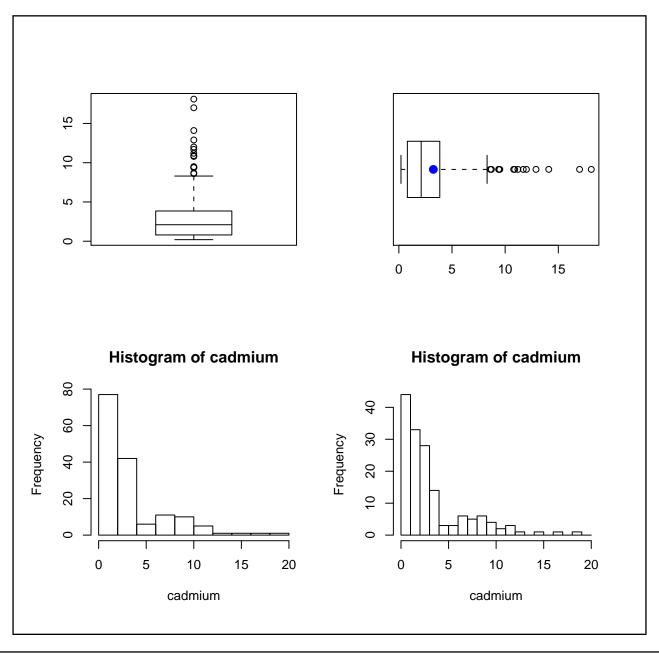


Example stem plot

```
> stem(cadmium)
 The decimal point is at the |
  1 | 0122222333333445555666777778888
  2 | 00011111244445556667777888899
  3 | 0011112245578999
  4 | 237
  5 | 568
  6 | 3568
  7 | 0013489
  8 | 122367
  9 | 4445
 10 | 89
 11 | 27
 12 I
      09
 13 |
 14 I
     1
 15 |
 16 I
 17 | 0
 18 | 1
```

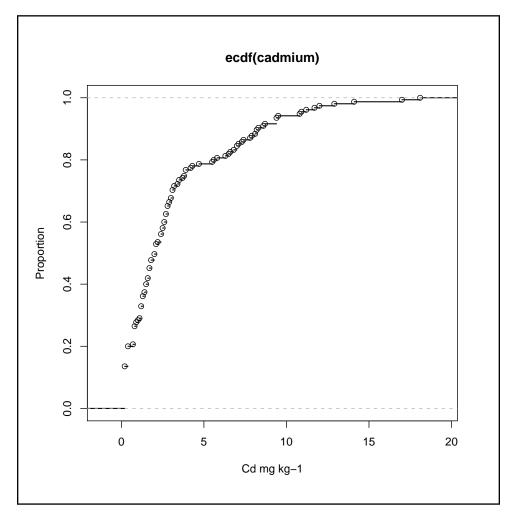


Example boxplots and histograms





Example empirical cumulative distribution plot





Summary statistics (1)

These summarize a single sample of a single variable

- 5-number summary (min, 1st Q, median, 3rd Q, max)
- Sample mean and variance

$$\overline{x} = \sum_{i=1}^{n} x_i$$
 $s_X^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \overline{x})^2$



Summary statistics (2)

Sample standard deviation (same units as mean), CV

$$s_X = \sqrt{s_X^2}$$
 $CV = \frac{s_X}{\overline{x}}$

```
> sd(cadmium)
[1] 3.523746
> sqrt(var(cadmium))
[1] 3.523746
> round((sqrt(var(cadmium))/mean(cadmium))*100,0)
[1] 109
```



Cautions

- The quantiles, including the median, are always meaningful
- The mean and variance are mathemtically meaningful, but not so useful unless the sample is "approximately" normal
- This imples one population (unimodal)

```
> quantile(cadmium, probs=seq(0, 1, .1))
             20%
  0 %
       10%
                   30%
                         40%
                               50%
                                     60%
                                          70%
                                                 80%
                                                       90%
                                                          100%
      0.20
           0.64 1.20 1.56 2.10 2.64 3.10
0.20
                                                5.64 8.26 18.10
```



Precision of the sample mean

Standard error of the mean: standard deviation adjusted by sample size

$$s_e = \frac{s_X}{\sqrt{n}}$$

- This is also written as $s_{\overline{X}}$
- Note that increasing sample size increases precision of the estimate (but as \sqrt{n} , not n)

```
> sd(cadmium)/sqrt(length(cadmium))
[1] 0.2830341
```



Confidence interval of the sample mean

- Estimated from sample mean and standard error, using the t distribution.
- Distribution the estimates of the mean is normal, even if the distribution of the variable isn't.

Test against null hypothesis of 0 (usually not very interesting):

```
> t.test(cadmium)
t = 11.4679, df = 154, p-value = < 2.2e-16
alternative hypothesis: true mean is not equal to 0
95 percent confidence interval:
   2.68668 3.80494
sample estimates:
mean of x
   3.24581</pre>
```



Test whether *less* than a **target value**; user must set α (confidence level):

```
> t.test(cadmium, alt="less", mu=3, conf.level = .99)
t = 0.8685, df = 154, p-value = 0.8068
alternative hypothesis: true mean is less than 3
99 percent confidence interval:
    -Inf 3.91116
sample estimates:
mean of x
3.24581
```

Note that in this case the confidence interval is *one sided*: from 3...3.91116; we don't care what the mean is if it's less than 3.



Populations & Outliers

- Most samples from "nature" are quite small
- Even if the assumption of one population with a normal distribution is true, by chance we can get extreme values
- How can we determine whether an "unusual" value is an outlier?
- How can we determine whether we have several populations?
- Answer: look for an underlying factor (co-variate), separate into sub-populations and test their difference



Topic: Bivariate EDA and correlation analysis

- "Bivariate": two variables which we suspect are related
- Question: what is the nature of the relation?
- Question: how strong is the relation?



Bivariate scatterplot

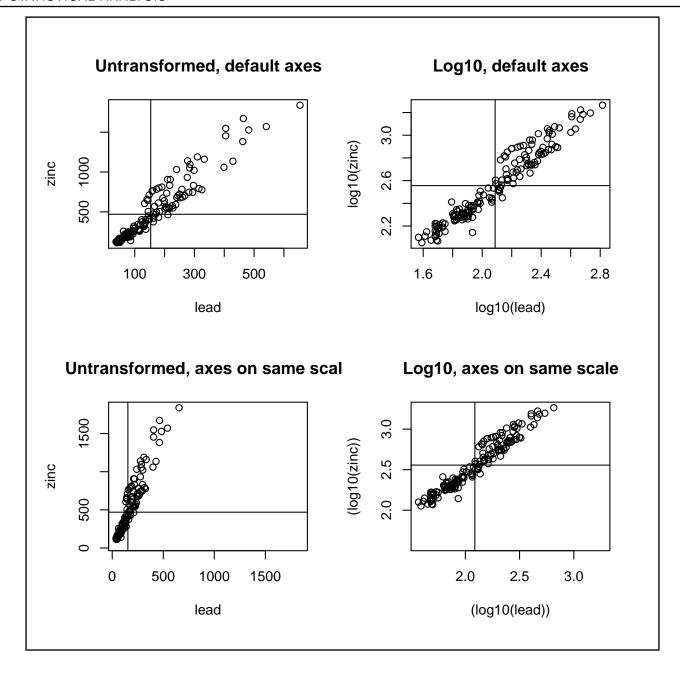
- Shows the relation of two variates in feature space (a plane made up of the two variables' ranges)
- Display two ways:
 - Non-standardized: with original values on the axes (and same zero);
 shows relative magnitudes
 - Standardized to zero sample means and unit variances: shows relative spreads
 - Note: some displays automatically scale the axes, so that non-standardized looks like standardized



Scatterplots of two heavy metals; automatic vs. same scales; also log-transformed; standardized and not.

```
> plot(lead, zinc)
> abline(v=mean(lead)); abline(h=mean(zinc))
> lim<-c(min(min(lead, zinc)), max(max(lead, zinc)))
> plot(lead, zinc, xlim=lim, ylim=lim)
> abline(v=mean(lead)); abline(h=mean(zinc))
> plot(log(lead), log(zinc))
> abline(v=mean(log(lead))); abline(h=mean(log(zinc)))
> plot(log(lead), log(zinc), xlim=log(lim), ylim=log(lim))
> abline(v=mean(log(lead))); abline(h=mean(log(zinc)))
> sdze<-function(x) { (x-mean(x))/sd(x) }
> plot(sdze(lead), sdze(zinc)); abline(h=0); abline(v=0)
> plot(sdze(log(lead)), sdze(log(zinc))); abline(h=0); abline(v=0)
```







Measuring the strength of a bivariate relation: theoretical

• The theoretical covariance of two variables X and Y

$$Cov(X,Y) = E\{(X - \mu_X)(Y - \mu_Y)\}$$
$$= \sigma_{XY}$$

• The *theoretical correlation coefficient*: covariance normalized by population standard deviations; range [-1...1]:

$$ho_{XY} = rac{\operatorname{Cov}(XY)}{\sigma_X \cdot \sigma_Y} \ = rac{\sigma_{XY}}{\sigma_X \cdot \sigma_Y}$$



Measuring the strength of a bivariate relation: estimate from sample

In practice, we estimate **population** covariance and correlation from a **sample**:

$$s_{xy} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \overline{x}) \cdot (y_i - \overline{y})$$

$$r_{xy} = \frac{s_{xy}}{s_x \cdot s_y}$$

$$= \frac{\sum (x_i - \overline{x}) \cdot \sum (y_i - \overline{y})}{\sqrt{\sum (x_i - \overline{x})^2 \cdot \sum (y_i - \overline{y})^2}}$$



Sample vs. population covariance and correlation

- Sample \bar{x} estimates population μ_X
- Sample s_x estimates population σ_X
- Sample r_{xy} estimates population ρ_{XY}



Example of correlation & confidence interval: positive, strong

This explains $0.955^2 = 0.912$ of the total variance.



Example of correlation & confidence interval: negative, weak

```
> cor.test(lead,dist.m)

Pearson's product-moment correlation

data: lead and dist.m

t = -8.9269, df = 153, p-value = 1.279e-15

alternative hypothesis: true correlation is not equal to 0

95 percent confidence interval:
    -0.6801118 -0.4710150

sample estimates:
    cor
    -0.5852087
```

This explains $-0.585^2 = 0.342$ of the total variance.



Topic: Regression

- A general term for modelling the distribution of one variable (the response or dependent) from ("on") another (the predictor or independent)
- This is only logical if we have a priori (non-statistical) reasons to believe in a causal relation
- Correlation: makes no assumptions about causation; both variables have the same logical status
- Regression: assumes one variable is the predictor and the other the response



Actual vs. fictional 'causality'

- Example: proportion of fine sand in a topsoil and subsoil layer
- Does one "cause" the other?
- Do they have a common cause?
- Can one be used to predict the other?
- Why would this be useful?



Simple linear regression (one predictor)

- Model: $y = \beta_0 + \beta_1 x + \varepsilon$
- β_0 : intercept, constant shift from \bar{x} to \bar{y}
- β_1 : slope, change in y for an equivalent change in x
- ε : error, or better, unexplained variation
- The parameters β_0 and β_1 are selected to minimize some summary measure of ε over all sample points



Simple regression (continued)

- Given the fitted model, we can **predict** at the original data points: \hat{y}_i ; these are called the **fitted values**
- Then we can compute the **deviations** of the fitted from the measured values: $\hat{e}_i = (\hat{y}_i y_i)$; these are called the **residuals**
- The deviations can be summarized to give an overall goodness-of-fit measure

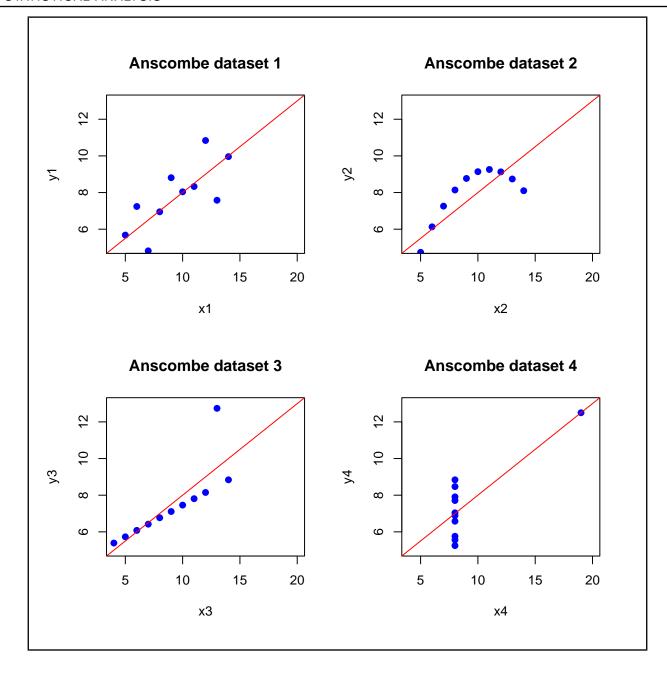


Look before you leap!

Anscombe developed four different bivariate datasets, all with the exact same correlation r = 0.81 and linear regression y = 3 + 0.5x:

- 1. bi-variate normal
- 2. quadratic
- 3. bi-variate normal with one outlier
- 4. one high-leverage point







Least squares estimates

- Compute the parameters to minimize the sum of the squared deviations
- Slope: $\beta_1 = s_{XY}/s_X^2$
- Note the similarly with covariance, except here we standardize by the *predictor* only, so the regression of *x* on *y* gives a different slope than that of *y* on *x*
- Intercept: To make the fitted and sample means co-incide: $\beta_0 = \overline{y} \beta_1 \overline{x}$



Sums of squares

- The regression partitions the variability in the sample into two parts:
 - 1 explained by the model
 - 2. not explained, left over, i.e. residual
- Note we always know the mean, so the total variability refers to the variability around the mean
- Question: how much more of the variability is explained by the model?
- Total SS = Regression SS + Residual SS

$$\sum_{i=1}^{n} (y_i - \overline{y})^2 = \sum_{i=1}^{n} (\hat{y}_i - \overline{y})^2 + \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

 The least squares estimate maximizes the Regression SS and minimizes the Residual SS



Analysis of Variance (ANOVA)

- Partition the total variance in a population into the model and residual
- If the model has more than one term, also partition the model variance into components due to each term
- Can be applied to any linear additive design specified by a model
- Each component can be tested for signficance vs. the null hypothesis that it does not contribute to the model fit



ANOVA for simple linear regression

- total sum of squared deviations is divided into model (regression) and error (residual) sums of squares
- Their ratio is the *coefficient of determination R*²
- These are each divided by their degrees of freedom to obtain the mean SS
- Their ratio is distributed as F and can be tested for significance

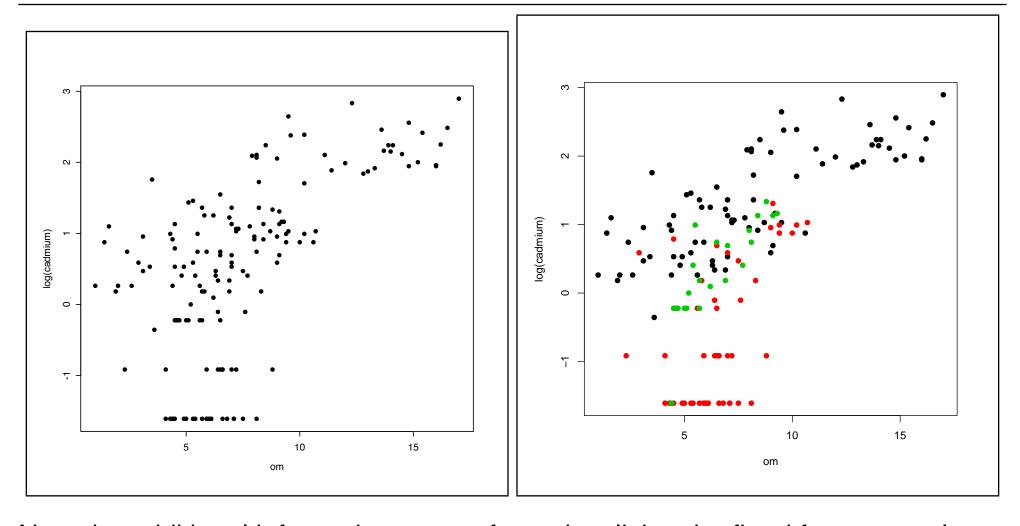


Bivariate analysis: heavy metals vs. organic matter

- Scatterplot
- Scatterplot by flood frequency
- Regression of metal on organic matter (why this order?)
- Same, including flood frequency in the model

```
> plot(om, log(cadmium))
> plot(om, log(cadmium), col=as.numeric(ffreq), cex=1.5, pch=20)
```





Note the additional information we get from visualising the flood frequency class.



Model: Regression of metal on organic matter

Highly-significant model, but organic matter content explains only about 35% of the variability of log(Cd).



Good fit vs. significant fit

- R^2 can be highly significant (reject null hypothesis of no relation), but ...
- ...the prediction can be poor
- In other words, only a "small" portion of the variance is explained by the model
- Two possiblities
 - 1. incorrect or incomplete model
 - (a) other factors are more predictive
 - (b) other factors can be included to improve the model
 - (c) form of the model is wrong
 - 2. correct model, noisy data
 - (a) imprecise **measurement** method ...
 - (b) ...or just an inherently variable process



Regression diagnostics

- Objective: to see if the regression truly represents the presumed relation
- Objective: to see if the computational methods are adequate
- Main tool: plot of standardized residuals vs. fitted values
- Numerical measures: leverage, large residuals



Examining the scatterplot with the fitted line

- Is there a trend in lack of fit? (further away in part of range)
 - ⋆ → a non-linear model
- Is there a trend in the spread?
 - * heteroscedasity (unequal variances) so linear modelling is invalid
- Are there high-leverage observations that, if eliminated, would substantially change the fit?
 - \star \rightarrow high *leverage*, isolated in the range and far from other points

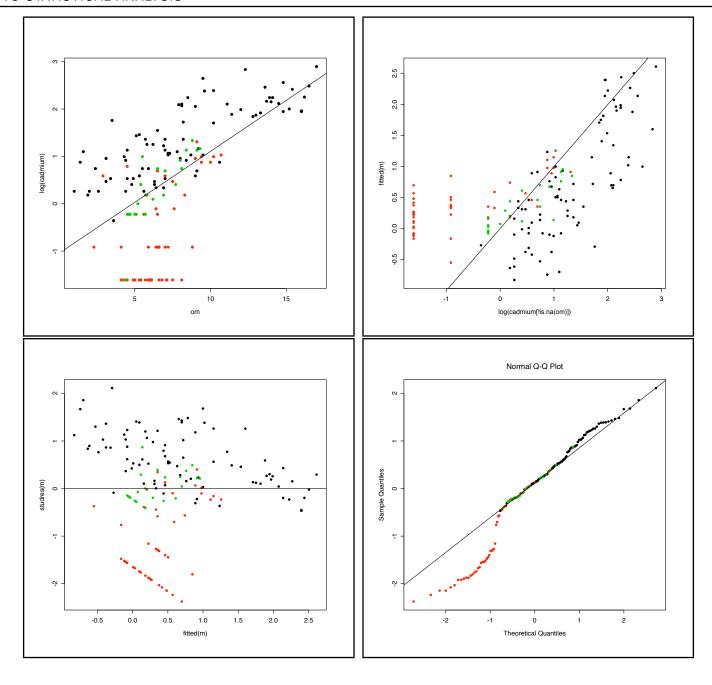


Model diagnostics: regression of metal on organic matter

```
> m<-lm(log(cadmium) ~ om)
> plot(om, log(cadmium), col=as.numeric(ffreq), cex=1.5, pch=20); abline(m)
> plot(log(cadmium[!is.na(om)]), fitted(m), col=as.numeric(ffreq), pch=20)
> abline(0,1)
> plot(fitted(m), studres(m), col=as.numeric(ffreq), pch=20)
> abline(h=0)
> qqnorm(studres(m), col=as.numeric(ffreq), pch=20);qqline(studres(m))
```

- We can see problems at the low metal concentrations. This is probably an artifact of the measurement precision at these levels (near or below the detection limit).
- These are almost all in flood frequency class 3 (rarely flooded).







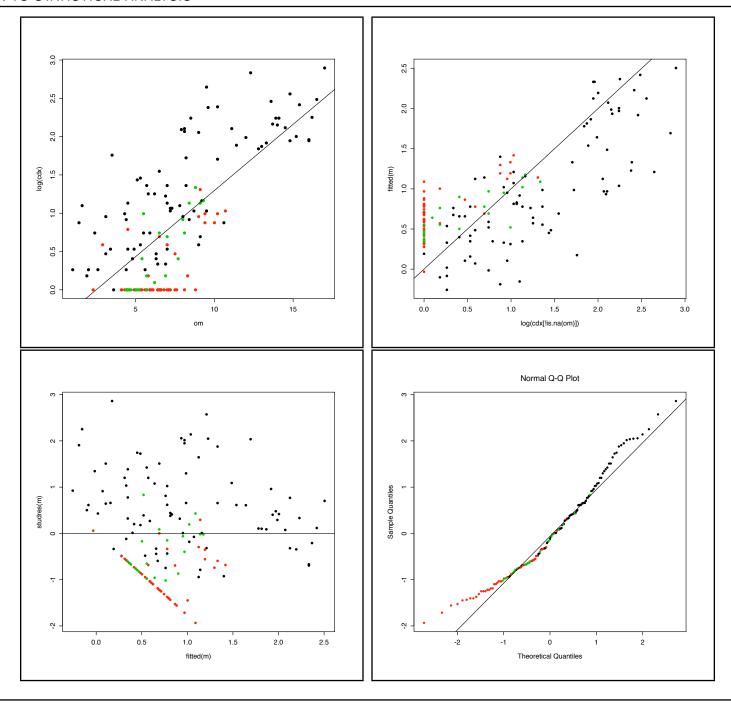
Revised model: Cd detection limit

Values of Cd below 1mg kg⁻¹ are unreliable; replace them all with 1mg kg⁻¹ and re-analyze:

```
> cdx<-ifelse(cadmium>1, cadmium, 1)
> plot(om, log(cdx), col=as.numeric(ffreq), cex=1.5, pch=20)
> m<-lm(log(cdx) ~ om); summary(m)</pre>
Residuals:
    Min
             10 Median
                             3Q
                                    Max
-1.0896 -0.4250 -0.0673 0.3527 1.5836
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.43030 0.11092 -3.879 0.000156 ***
             0.17272 0.01349 12.806 < 2e-16 ***
om
Residual standard error: 0.5709 on 151 degrees of freedom
Multiple R-Squared: 0.5206, Adjusted R-squared: 0.5174
F-statistic:
               164 on 1 and 151 DF, p-value: < 2.2e-16
> abline(m)
> plot(log(cdx[!is.na(om)]), fitted(m), col=as.numeric(ffreq), pch=20); abline(0,1)
> plot(fitted(m), studres(m), col=as.numeric(ffreq), pch=20); abline(h=0)
> gqnorm(studres(m),col=as.numeric(ffreq),pch=20); gqline(studres(m))
```

Much higher R^2 and better diagnostics. Still, there is a lot of spread at any value of the predictor (organic matter).







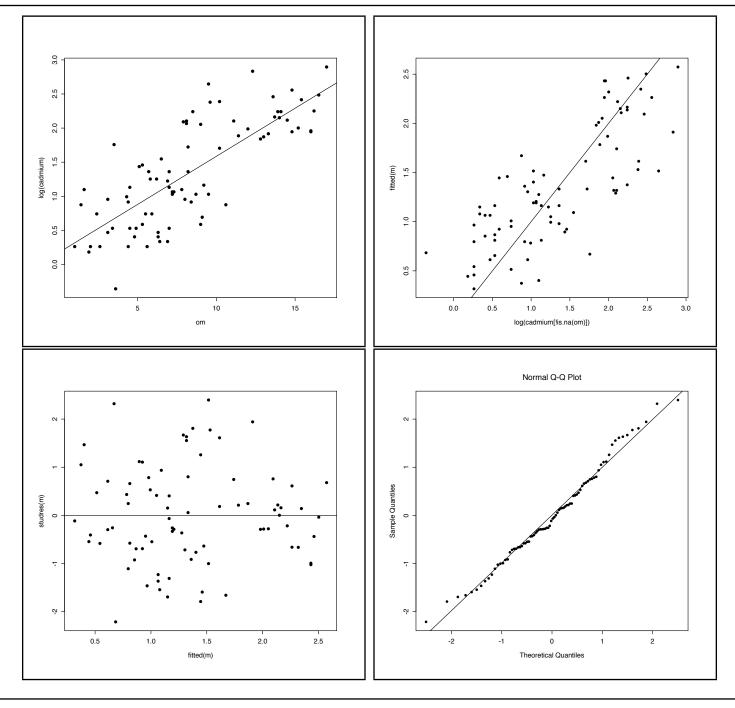
Revised model: flood class 1

The relation looks more consistent in the frequently-flooded soils; re-analyze this subset.

```
> meuse.1<-meuse[ffreq==1,]; attach(meuse.1)</pre>
> plot(om, log(cadmium), cex=1.6, pch=20)
> m<-lm(log(cadmium) ~ om); summary(m)</pre>
Residuals:
    Min
                 Median
                                30
              10
                                       Max
-1.04064 -0.31782 -0.04348 0.32210 1.13034
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.17639 0.11999 1.47 0.145
            \circ m
Residual standard error: 0.4888 on 80 degrees of freedom
Multiple R-Squared: 0.6003, Adjusted R-squared: 0.5954
F-statistic: 120.2 on 1 and 80 DF, p-value: < 2.2e-16
> abline(m)
> plot(log(cadmium[!is.na(om)]), fitted(m)); abline(0,1)
> plot(fitted(m), studres(m)); abline(h=0)
> gqnorm(studres(m)); gqline(studres(m))
```

Still higher R^2 and excellent diagnostics. There is still a lot of spread at any value of the predictor (organic matter), so OM is not an efficient predictor of Cd.







Categorical ANOVA

- Model the response by a categorical variable (nominal); ordinal variables are treated as nominal
- Model: $y = \beta_0 + \beta_j x + \varepsilon$; where each observation x is multiplied by the $beta_j$ corresponding to the class to which it belongs (of n classes)
- The β_i represent the deviations of each class mean from the grand mean



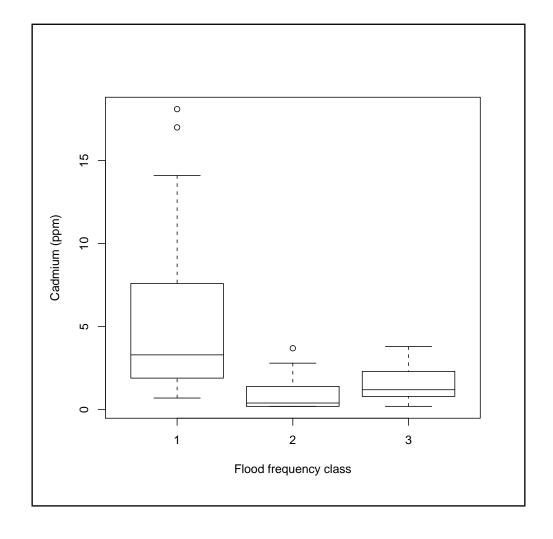
Example: Meuse soil pollution

- Question: do metals depend on flood frequency (3 of these)
- EDA: categorical boxplots
- Analysis: one-way ANOVA on the frequency



Categorical EDA

> boxplot(cadmium ~ ffreq,xlab="Flood frequency class",ylab="Cadmium (ppm)")





Example ANOVA

```
> m<-lm(log(cadmium) ~ ffreq)</pre>
> summary(m)
Residuals:
       1Q Median 3Q
   Min
                                  Max
-1.8512 -0.7968 -0.1960 0.7331 1.9354
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.32743 0.09351 14.196 < 2e-16 ***
ffreq2
           -1.95451 0.15506 -12.605 < 2e-16 ***
           -1.08566 0.20168 -5.383 2.72e-07 ***
ffreq3
Residual standard error: 0.857 on 152 degrees of freedom
Multiple R-Squared: 0.5169, Adjusted R-squared: 0.5105
F-statistic: 81.31 on 2 and 152 DF, p-value: < 2.2e-16
```



Difference between classes

All per-pair class differences are significant (confidence interval does not include zero).



Non-parametric statistics

A **non-parametric** statistic is one that does not assume any underlying data distribution.

For example:

- a mean is an estimate of a parameter of location of some assumed distribution (e.g.mid-point of normal, expected proportion of success in a binomial, . . .)
- a median is simply the value at which half the samples are smaller and half larger, without knowing anything about the distribution underlying the process which produced the sample.

So "non-parametric" inferential methods are those that make no assumptions about the distribution of the data values, only their order (rank).



Non-parametric statistics: Correlation

As an example of the non-parameteric approach, consider the measure of association between two variables, commonly called *correlation* ('co-relation').

The standard measure is *parametric*, i.e. the Pearson's Product Moment Correlation (PPMC); this is computed from the sample covariance of the two variables:

$$Cov(X,Y) = \frac{1}{n-1} \sum_{i=1}^{n} \{(x_i - \bar{x})(y_i - \bar{y})\}$$

Then the sample Pearson's correlation coefficient is computed as:

$$r_{XY} = \operatorname{Cov}(X,Y)/s_X \cdot s_Y$$

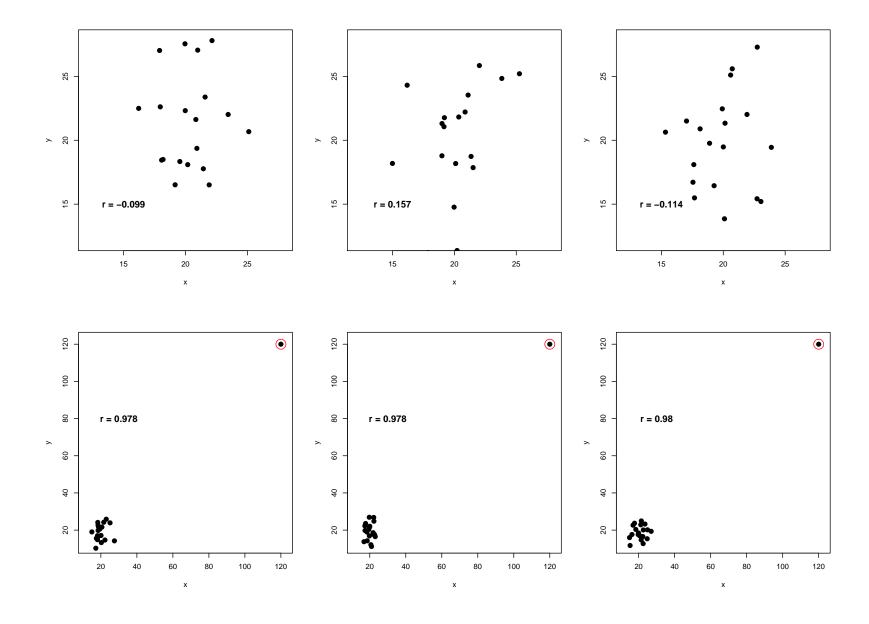


Parametric correlation – example of inappropriate use

Consider the following two cases: (1) 20 bivariate normal samples that should be uncorrelated; (2) same, but with one value replaced by a very high value (no longer a normal distribution).

```
n<-20
par(mfrow=c(2,3))
for (i in 1:3)
  { x<-rnorm(n, 20, 3); y<-rnorm(n, 20, 4);
    plot(x,y, pch=20, cex=2, xlim=c(12,28), ylim=c(12,28));
    text(15,15, paste("r =",round(cor(x,y),3)), font=2, cex=1.2)
}
for (i in 1:3)
  { x<-c(rnorm((n-1), 20, 3), 120); y<-c(rnorm((n-1), 20, 4), 120);
    plot(x,y, pch=20, cex=2, xlim=c(12, 122), ylim=c(12, 122));
    points(120, 120, col="red", cex=3);
    text(30,80, paste("r =",round(cor(x,y),3)), font=2, cex=1.2)
}</pre>
```







Non-parametric correlation

The solution here is to use a method such as *Spearman's* correlation, which correlates the **ranks**, not the **values**; therefore the distribution ("gaps between values") has no influence.

From numbers to ranks:

```
> n<-10
> (x<-rnorm(n, 20, 4))
 [1] 15.1179 23.7801 21.2801 21.5191 23.0096 18.5065 19.1448 24.9254 29.3211
[10] 14.1453
> (ix<-(sort(x, index=T)$ix))
 [1] 10 1 6 7 3 4 5 2 8 9</pre>
```

If we change the largest of these to any large value, the rank does not change:

```
> x[ix[n]]<-120; x
[1] 15.1179 23.7801 21.2801 21.5191 23.0096 18.5065 19.1448 24.9254
[9] 120.0000 14.1453
> (ix<-(sort(x, index=T)$ix))
[1] 10 1 6 7 3 4 5 2 8 9</pre>
```



Compare the two correlation coefficients:

```
pearsons<-vector(); spearmans<-vector()</pre>
> n < -10
> for (i in 1:n)
 \{ x < -rnorm(n, 20, 4); y < -rnorm(n, 20, 4); \}
    pearsons[i] < -cor(x, y);
    spearmans[i] <-cor(x,y, method="spearman") }</pre>
> round(pearsons, 2); round(spearmans, 2)
 [1] -0.29 -0.02 -0.49 -0.01 -0.17 0.16 0.06 -0.07 -0.11 0.37
 [1] 0.32 0.16 -0.25 0.01 0.35 -0.42 0.03 -0.33 0.68 -0.12
> for (i in 1:n)
 \{x < -c(rnorm((n-1), 20, 4), 120); y < -c(rnorm((n-1), 20, 4), 120); \}
    pearsons[i] < -cor(x, y);
    spearmans[i] <-cor(x,y, method="spearman") }</pre>
> round(pearsons, 2); round(spearmans, 2)
 [1] 0.25 0.08 0.49 0.03 0.61 -0.04 0.36 0.26 -0.25 0.36
```

The Pearson's (parametric) coefficient is completely changed by the one high-valued pair, whereas the Spearman's is unaffected.



Other non-parametric methods

- t-test for equivalence of means → Mann-Whitney test for equivalence of medians
- One-way ANOVA → Kruskal-Wallis
- χ^2 goodness-of-fit \rightarrow **Kolmogorov-Smirnov** goodness-of-fit

