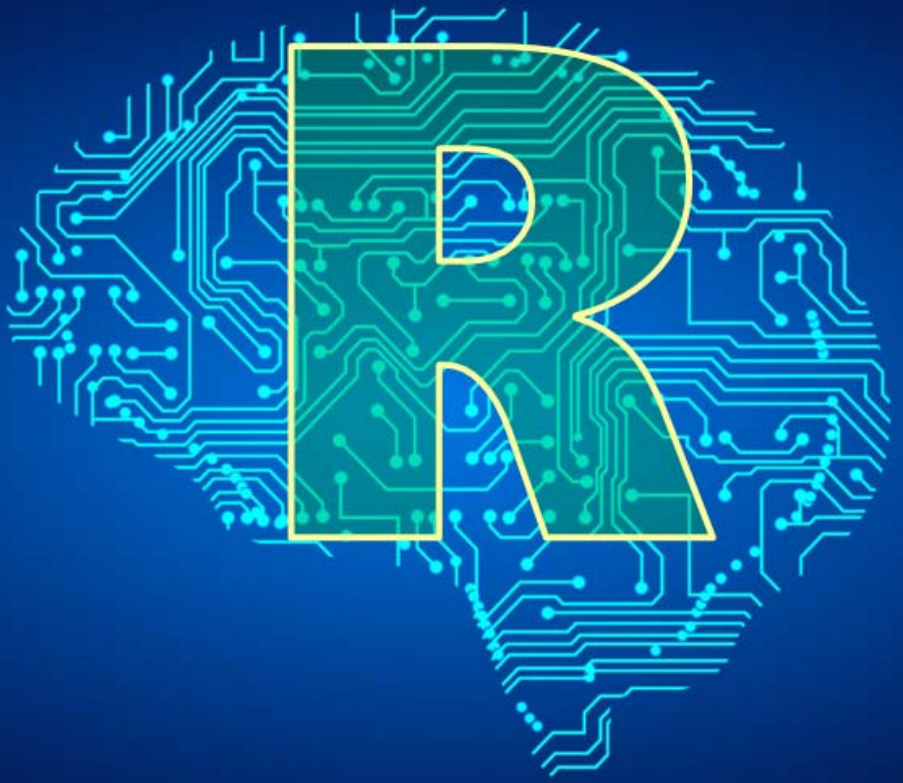
D2-3

台灣人工智慧學校



資料轉換

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本章大綱

- Why Data Transformations?
- Data Discretization, Reasons for Non-normality
- Common Transformations
  - Range，Reciprocal, Square Root, **Log**, Power Transformation , **Box-Cox Transformations**.
  - 範例: BUPA Liver Data Set
- Transformations for Proportions and Percents: Logit Transformation
- Variance Stabilizing Transformations
- Standardization
  - 範例: Microarray Data of Yeast Cell Cycle, Crab Data
- Species Data Transformation: The Doubs Fish Data
- Sphering for Multivariate Variables
- Which Transformation?
- Normalization for Microarray Gene Expression Data

Classical (Numerical) Data Table

*j*th variables

subjects

*i*th sample

UID	alpha0	alpha7	alpha14	alpha21	alpha28	alpha35	alpha42
YAR007C	-0.48	-0.42	0.87	0.92	0.67	-0.18	-0.35
YBL035C	-0.39	-0.58	1.08	1.21	0.52	-0.3	
YBR023C	0.87	0.25	-0.17	0.18	-0.13	-0.44	-0.13
YBR067C	1.57	1.03	1.22	0.31	0.16	-0.49	-1.02
YBR088C	-1.15	-0.86	1.21	1.62	1.12	0.16	-0.44
YBR278W	0.04	-0.12	0.31	0.16	0.17	-0.06	0.08
YCL055W	2.95	0.45	-0.4	-0.66	-0.59	-0.38	-0.76
YDL003W	-1.22	-0.74	1.34	1.5	0.63	0.29	-0.55
YDL055C	-0.73	-1.06	-0.79	-0.02	0.16	0.44	0.03
YDL102W	-0.58	-0.4	0.13	0.58	-0.09	0.02	-0.45
YDL164C	-0.5	-0.42	0.66	1.05	0.68	0.06	0.01
YDL197C	-0.86	-0.29	0.42	0.46	0.3	0.1	-0.63
YDL227C	-0.16	0.2877	0.17	-0.28	-0.02	-0.55	-0.04
YDR052C	-0.36	-0.03	-0.03	-0.08	-0.23	-0.25	-0.21
YDR097C	-0.72	-0.85	0.54	1.04	0.84	0.24	-0.64
YDR113C	-0.78	-0.52	0.26	0.2	0.48	0.48	0.27
YDR309C	0.6	-0.55	0.41	0.45	0.18	-0.66	-1.02
YDR356W	-0.2	-0.67	0.13	0.1	0.38	0.44	0.05
YER001W	-2.29	-0.635739	0.77	1.6	0.53	0.55	-0.38
YER070W	-1.46	-0.76	1.08	1.5	0.74	0.47	-0.7
YER095W	-0.57	0.42	1.03	1.35	0.64	0.42	-0.4
YGL163C	-0.11	0.13	0.41	0.6	0.23	0.31	0.19
YGL225W	-1.08	-0.99	-0.16	0.2	0.61	0.37	0.1
YGR109C	-1.79	0.9449	2.13	1.75	0.23	0.15	-0.66

transformation for each row

transformation for each column

transformation for both rows and columns

Data Transformations

- A transformation of a set of data points $x_1, x_2, \ldots, x_n$ is a function T that substitutes each observation x_i with a new value $T(x_i)$.

- Transformations should have the following properties:
  - The **order** of the data is preserved by the transformation.
  - They are **continuous functions** guaranteeing that points that are close together in raw form are also close together using their transformed values, relative to the scale used.
  - They are **smooth functions** that have derivatives of all orders, and they are specified by elementary functions.

- In EDA, we might want to change the shape of data (**reexpressed**) to facilitate visualization, smoothing, and other analyses.

Why Data Transformations? (1/2)

- Many statistical procedures make two assumptions that are relevant to data transformation:
  - (a) the variables (or their error terms) are **normally distributed**.
  - (b) homoscedasticity or **homogeneity of variance**, meaning that the variance of the variable remains constant over the observed range of some other variable.

- In regression analyses the assumption (b) is that the variance around the regression line is constant across the entire observed range of data.
- In ANOVA analyses, the assumption (b) is that the variance in one cell is not significantly different from that of other cells.

- In some cases, transforming the data will make it **fit the assumptions** better.

Why Data Transformations? (2/2)

- Transforms are usually applied:
  - so that the data appear to more closely **meet the assumptions** of a statistical inference procedure that is to be applied,
  - to make it **easier to visualize** (appearance of graphs),
  - to improve **interpretability**, even if no formal statistical analysis or visualization is to be performed.
  - to make descriptors that have been measured in **different units comparable**,
  - to make the relationships among **variables linear**,
  - to modify the **weights** of the variables or objects (e.g. give the same length (or norm) to all object vectors)
  - to **code** categorical variables into dummy binary variables.

- Guidance for how data should be transformed, or whether a transformation should be applied at all, should come from the particular statistical analysis to be performed.

Data Transformation

- **Smoothing**: This uses binning, regression, and clustering to remove noise from the data.
- **Attribute construction**: In this routine, new attributes are constructed and added from the given set of attributes.
- **Aggregation**: In this summary or aggregation, operations are performed on the data.
- **Normalization**: Here, the attribute data is scaled so as to fall within a smaller range.
- **Discretization**: In this routine, the raw values of a numeric attribute are replaced by interval label or conceptual label.
- **Concept hierarchy generation for nominal data**: Here, attributes can be generalized to higher level concepts.

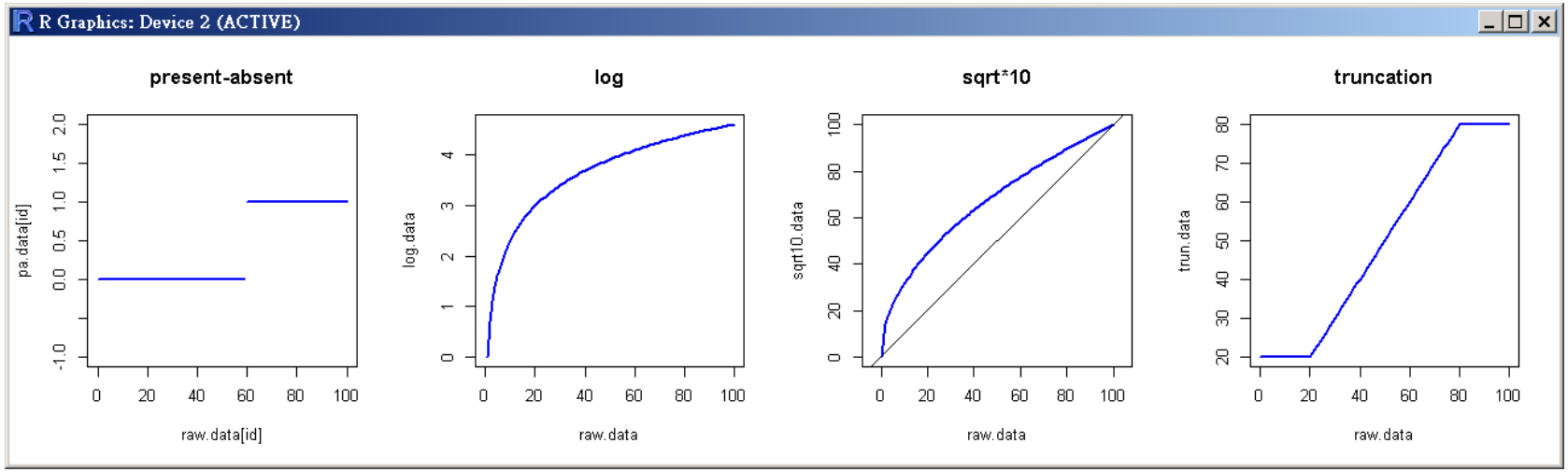
Data Discretization

- Data discretization transforms numeric data by mapping values to interval or concept labels.
- **by binning**: This is a top-down unsupervised splitting technique based on a specified number of bins.
- **by histogram analysis**: In this technique, a histogram partitions the values of an attribute into disjoint ranges called buckets or bins. It is also an unsupervised method.
- **by cluster analysis**: In this technique, a clustering algorithm can be applied to discretize a numerical attribute by partitioning the values of that attribute into clusters or groups.
- **by decision tree analysis**: Here, a decision tree employs a top-down splitting approach; it is a supervised method. To discretize a numeric attribute, the method selects the value of the attribute that has minimum entropy as a split-point, and recursively partitions the resulting intervals to arrive at a hierarchical discretization.
- **by correlation analysis**: This employs a bottom-up approach by finding the best neighboring intervals and then merging them to form larger intervals, recursively. It is supervised method.

Common Transformations (1/3)

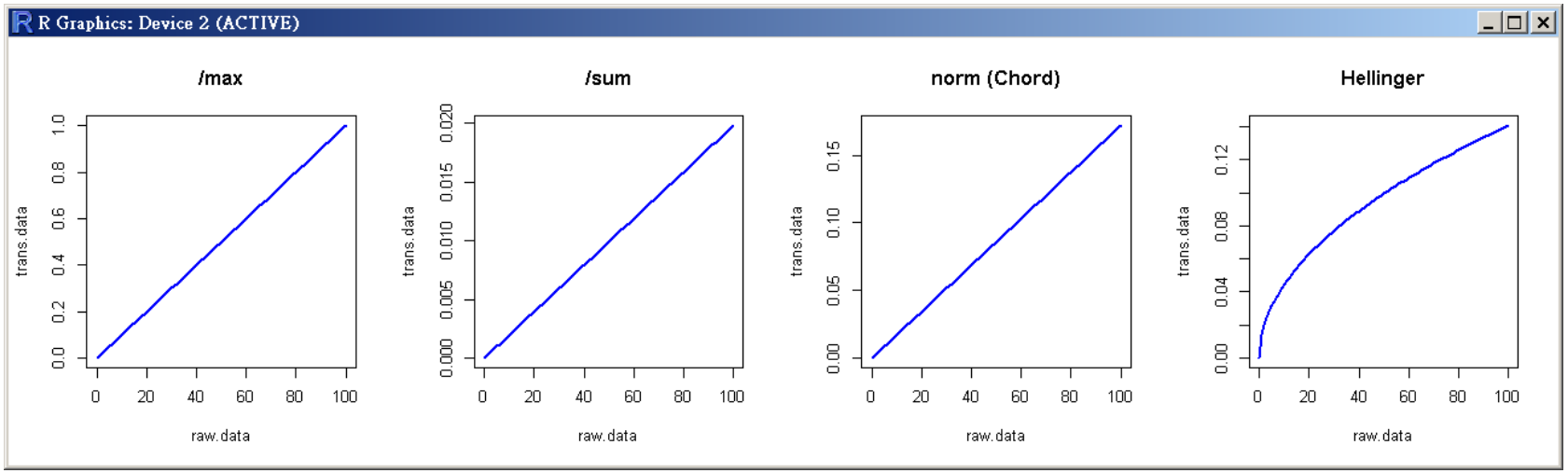
```
> par(mfrow=c(1,4))
> raw.data <- 0:100
> pa.data <- ifelse(raw.data >= 60, 1, 0)
> id <- which(pa.data==1)
> plot(raw.data[id], pa.data[id], main="present-absent",
+ type="l", lwd=2, col="blue", ylim=c(-1, 2), xlim=c(0, 100))
> points(raw.data[-id], pa.data[-id], type="l", lwd=2, col="blue")
>
> log.data <- log(raw.data)
> plot(raw.data, log.data, main="log", type="l", lwd=2, col="blue")
>
> sqrt10.data <- sqrt(raw.data)*10
> plot(raw.data, sqrt10.data, main="sqrt*10", type="l", lwd=2, col="blue", asp=1)
> abline(a=0, b=1)
>
> trun.data <- ifelse(raw.data >= 80, 80, ifelse(raw.data < 20, 20, raw.data))
> plot(raw.data, trun.data, main="truncation", type="l", lwd=2, col="blue")
```

NOTE:
```
apply(raw.data.matrix, 2, log)
apply(raw.data.matrix, 2, function(x) sqrt(x)*10)
apply(raw.data.matrix, 2, myfun)
```



Common Transformations (2/3)

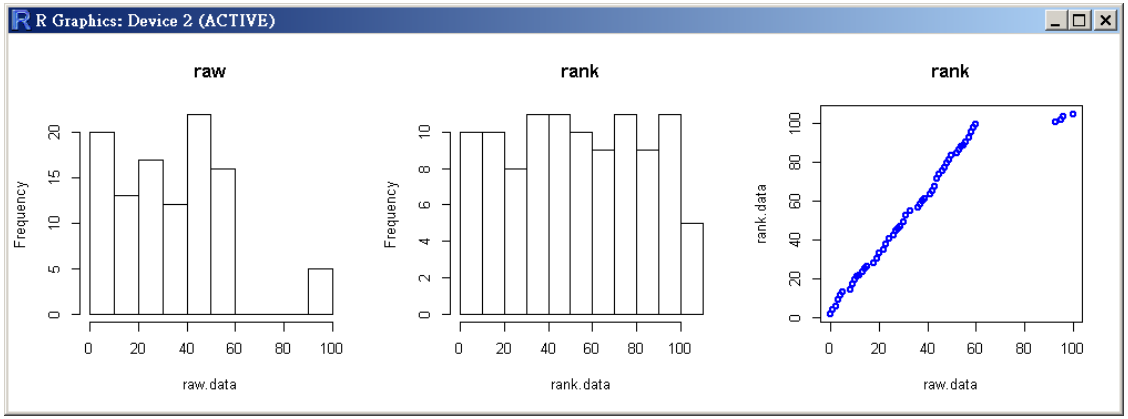
```
> par(mfrow=c(1,4))
> raw.data <- 0:100
> trans.data <- raw.data/max(raw.data)
> plot(raw.data, trans.data, main="/max", type="l", lwd=2, col="blue")
>
> trans.data <- raw.data/sum(raw.data)  #Species profile transformation
> plot(raw.data, trans.data, main="/sum", type="l", lwd=2, col="blue")
>
> trans.data <- raw.data/sqrt(sum(raw.data^2)) #length of 1, Chord transformation
> plot(raw.data, trans.data, main="norm (Chord)", type="l", lwd=2, col="blue")
>
> trans.data <- sqrt(raw.data/sum(raw.data)) #Hellinger transformation
> plot(raw.data, trans.data, main="Hellinger", type="l", lwd=2, col="blue")
```



Other Transformations for community composition data: Chi-square distance transformation, Chi-square metric transformation

Common Transformations (3/3)

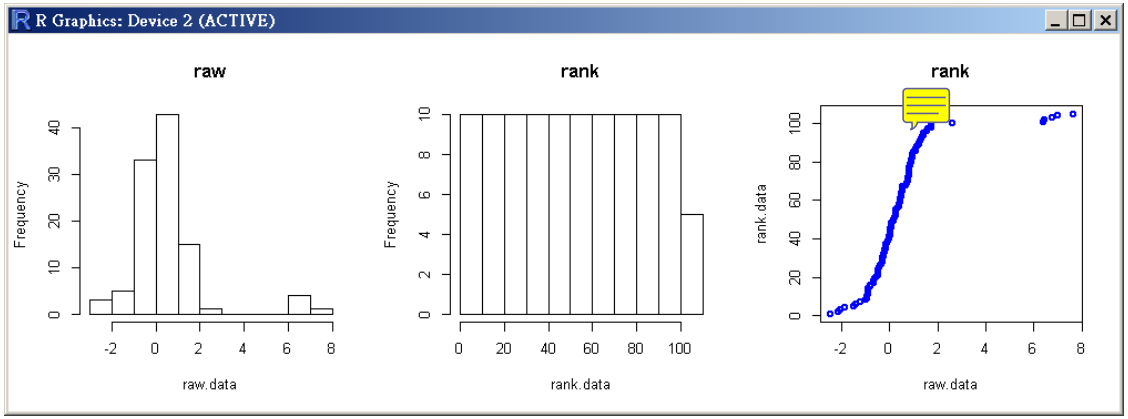
```
> par(mfrow=c(1,3)); set.seed(12345)
> raw.data <- c(sample(0:60, 100, replace=T), sample(90:100, 5, replace=T))
> rank.data <- rank(raw.data)
> hist(raw.data, main="raw")
> hist(rank.data, main="rank")
> plot(raw.data, rank.data, main="rank", lwd=2, col="blue")
>
> raw.data <- c(rnorm(100), rnorm(5)+ 2*sqrt(qchisq(0.975, 5)))
...
```



Outlier values $\sim$

$$2 \times \sqrt{\chi^2_{0.975,p}} + N(0,1)$$

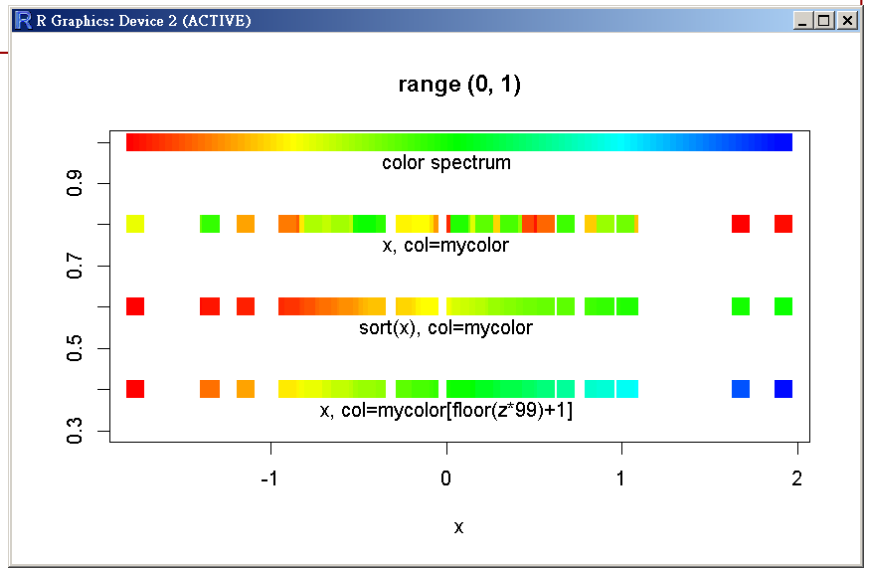
```
> qchisq(0.975,5)
[1] 12.83250
```



Transformation Using the Range

- use the range of the variable as the divisor:
  - $z = (x-min(x))/(max(x)-min(x))$, is **bounded by zero and one**, with at least one observed value at each of the end points.

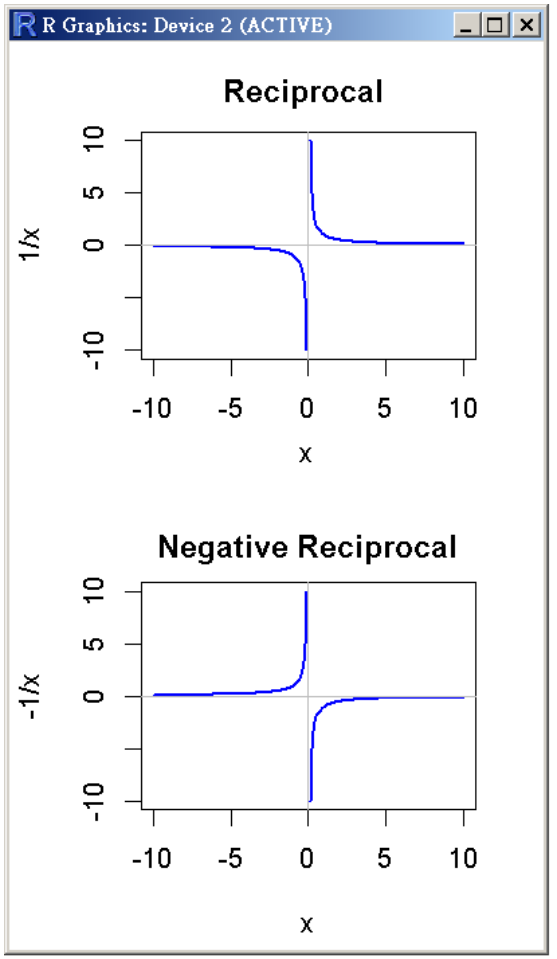
```
x <- rnorm(50)
mycolor <- rainbow(150)[1:100]
z <- (x-min(x))/(max(x)-min(x))
plot(x, rep(1, length(x)), main="range (0, 1)", type="n", ylab="", ylim=c(0.3,1))
points(c(seq(min(x), max(x), length.out=100)), rep(1, 100), col=mycolor, cex=2, pch=15)
text(0, 0.95, "color spectrum")
points(x, rep(0.8, length(x)), col=mycolor, cex=2, pch=15)
text(0, 0.75, "x, col=mycolor")
points(sort(x), rep(0.6, length(x)), col=mycolor, cex=2, pch=15)
text(0, 0.55, "sort(x), col=mycolor")
points(x, rep(0.4, length(x)), col=mycolor[floor(z*99)+1], cex=2, pch=15)
text(0, 0.35, "x, col=mycolor[floor(z*99)+1]")
```



- The transformed variate is a linear function of the other one, so data standardized using these transformations will result in identical Euclidean distances.

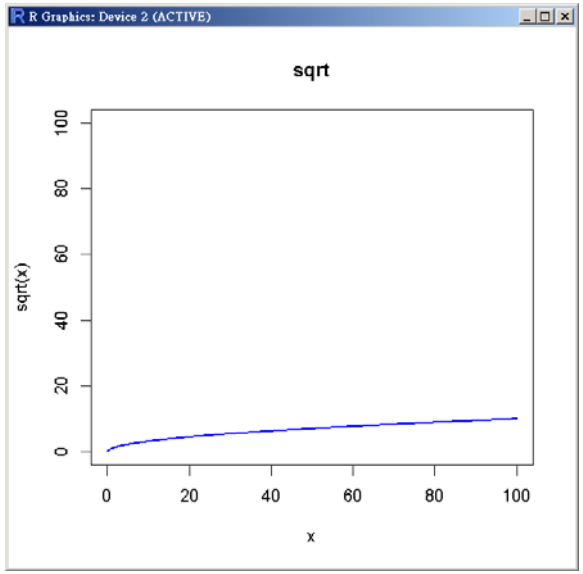
The Reciprocal Transformation

- The **reciprocal**, x to $1/x$, with its sibling the **negative reciprocal**, x to $-1/x$, is a very strong transformation with a drastic effect on distribution shape.
- The reciprocal reverses order among values of the same sign: largest becomes smallest, etc.
- The negative reciprocal preserves order among values of the same sign.
- (In practice, we might want to multiply or divide the results of taking the reciprocal by some constant, such as 1000 or 10000, to get numbers that are easy to manage, but that itself has no effect on skewness or linearity.)
- The reciprocal of a **ratio** may be interpreted as easily as the ratio itself:
  - population density (people per unit area) becomes area per person;
  - persons per doctor becomes doctors per person;
  - rates of erosion become time to erode a unit depth.

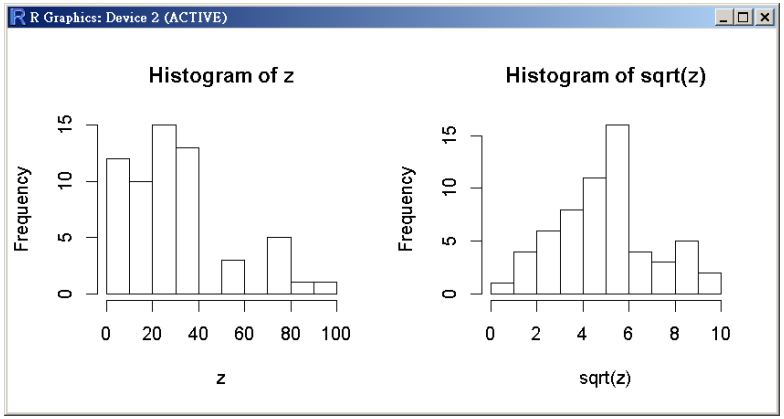


The Square Root Transformation

- The square root, x to $x^{1/2} = sqrt(x)$, is a transformation with a moderate effect on distribution shape: it is weaker than the logarithm and the cube root.
- It is used for **reducing right skewness**, and also has the advantage that it can be applied to zero values.
- Note that the square root of an area has the units of a length. It is commonly applied to **counted data**, especially if the value are mostly rather small.




```
> x <- sample(0:40, 50, replace=T)
> y <- sample(40:100, 10)
> z <- c(x,y)
> par(mfrow=c(1,2))
> hist(z)
> hist(sqrt(z))
```



範例: Software Inspection Data

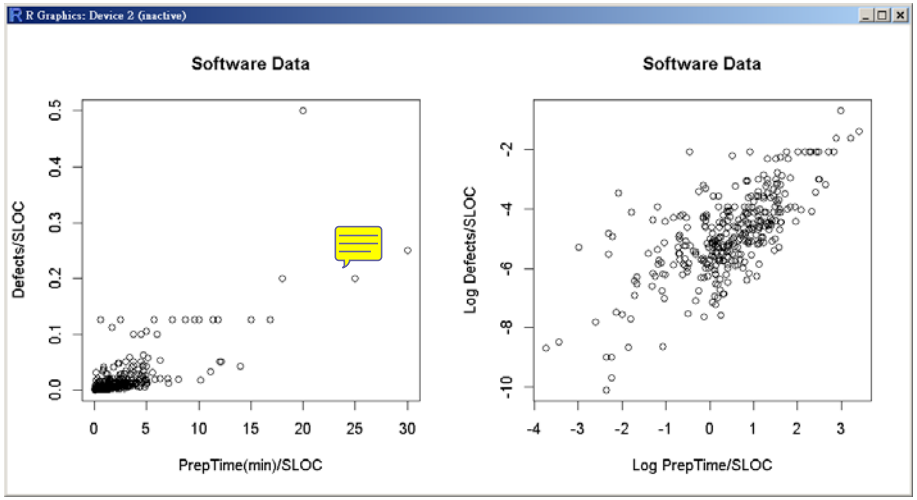
- The data were collected in response to efforts for process improvement in software testing by code inspection.
- First they look for inconsistencies, logical errors, etc., and decide what they perceive as defects. The defect types include compatibility, design, human-factors, standards, and others.
- The variables are normalized by the size of the inspection (the number of pages or SLOC (single lines of code): the preparation time in minutes (**prepage, prepsloc**), the total work hours in minutes for the meeting (**mtgsloc**), and the number of defects found (**defpage**, **defsloc**).
- Interested in: understanding the relationship between the inspection time and the number of defects found.

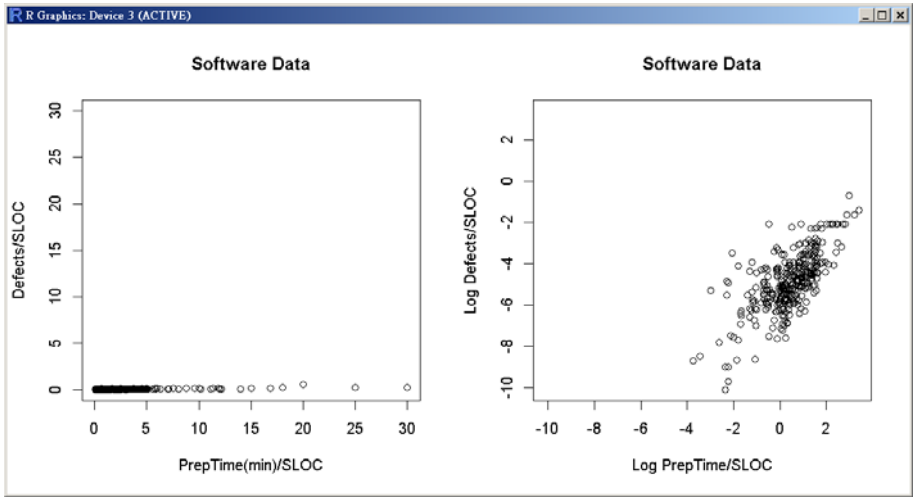
```
> library('R.matlab')
> data <- readMat("software.mat")
> print(data)
...
> str(data)
List of 5
 $ prepsloc: num [1:426, 1] 0.485 0.54 0.54 0.311 0.438 ...
 $ defsloc : num [1:426, 1] 0.005 0.002 0.002 0.00328 0.00278 ...
 $ mtgsloc : num [1:426, 1] 0.075 0.06 0.06 0.2787 0.0417 ...
 $ prepage : num [1:491, 1] 6.15 1.47 1.47 5.06 5.06 ...
 $ defpage : num [1:491, 1] 0.0385 0.0267 0.0133 0.0128 0.0385 ...
```

Log Transformations (1/3)

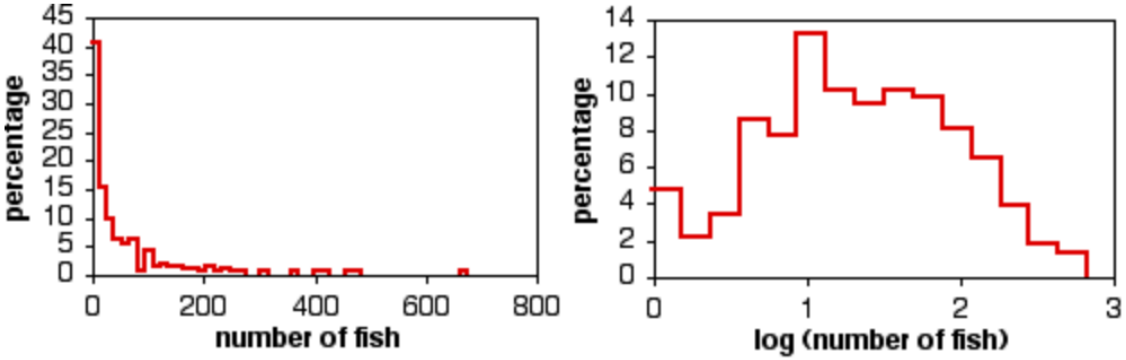
- The data are skewed, and the relationship between the variables is difficult to understand.
- We apply a log transform to both variables.
- In any application of EDA, the analyst should go back to the subject area and consult domain experts to verify and help interpret the results.

```
par(mfrow=c(1,2))
xylim <- range(data$prepsloc, data$defsloc)
plot(data$prepsloc, data$defsloc, xlab="PrepTime(min)/SLOC", ylab="Defects/SLOC",
main="Software Data", xlim=xylim, ylim=xylim)
logxylim <- range(log(data$prepsloc), log(data$defsloc))
plot(log(data$prepsloc), log(data$defsloc), xlab="Log PrepTime/SLOC",
ylab="Log Defects/SLOC", main="Software Data", xlim=logxylim, ylim=logxylim)
```





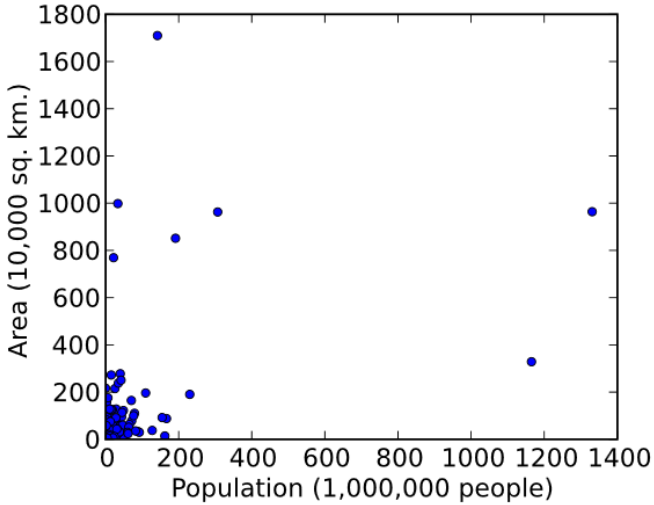
Log Transformations (2/3)

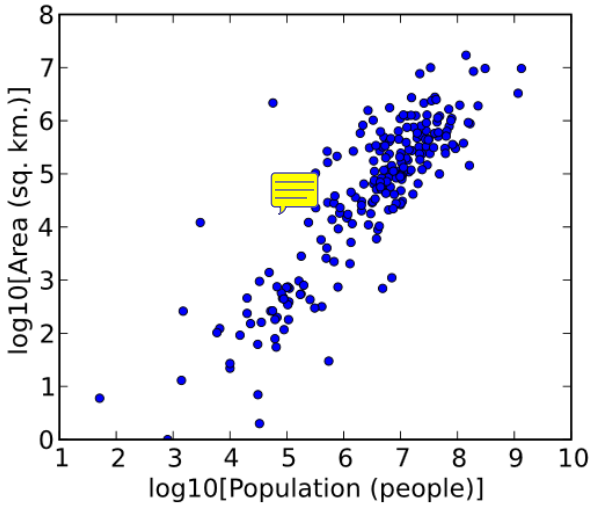


Histograms of number of Eastern mudminnows per 75 m section of stream (samples with 0 mudminnows excluded). Untransformed data on left, log-transformed data on right.

Source:
http://www.biostathandbook.com/transformation.html

The areas of the sovereign states and dependent territories in the world are plotted on the vertical axis against their populations on the horizontal axis.





https://en.wikipedia.org/wiki/Data_transformation_%28statistics%29

Log Transformations (3/3)

- Consider ratios $y = p/q$ where p and q are both positive in practice. Examples are
  - males / females;
  - dependents / workers;
  - downstream length / downvalley length.

- Then y is somewhere between 0 and infinity, or between 1 and infinity. (If $p = q$, then $y = 1$.) Such definitions often lead to **skewed data**, because there is a clear lower limit and no clear upper limit.

- The logarithm, $\log y = \log (p/q) = \log p - \log q$, is somewhere between -infinity and infinity and $p = q$ means that $\log y = 0$. Hence the logarithm of such a ratio is likely to be more symmetrically distributed.

Log Transformations: How to Handle Negative Data Values?

- In many cases, the variable of interest is positive and the log transformation is immediately applicable. However, some quantities (for example, profit) might contain a few negative values. How do you handle negative values if you want to log-transform the data?

Solution 1: Translate, then Transform

- $log(Y+a)$ where a is the constant.
- Choose a so that $min(Y+a)$ is a very small positive number (like 0.001).
- Choose a so that $min(Y+a) = 1$.
- *cond(x <= 0, -ln(-x + 1), ln(x + 1))*

Solution 2: Use Missing Values

- A criticism of the previous method is that some practicing statisticians don't like to add an arbitrary constant to the data.
- They argue that a better way to handle negative values is to use missing values for the logarithm of a nonpositive number.

Power Transformation (1/2)

- For data vectors $(y_1,\ldots, y_n)$ in which each $y_i > 0$, the power transform is

$$y_i^{(\lambda)} = \begin{cases} \dfrac{y_i^{\lambda} - 1}{\lambda(\mathrm{GM}(y))^{\lambda-1}}, & \text{if } \lambda \neq 0 \\ \mathrm{GM}(y) \ln y_i, & \text{if } \lambda = 0 \end{cases}$$

where

$$\mathrm{GM}(y) = (y_1 \cdots y_n)^{1/n}$$

is the geometric mean of the observations $y_1, \ldots, y_n$.

- The power transform corresponds to **a family of functions** that are applied to create a **monotonic transformation** of data using power functions.
- This transformation is used to **stabilize variance**, make the data more normal distribution-like, improve the validity of measures of association such as the Pearson correlation between variables and for other data stabilization procedures.
- When both negative and positive values are observed, it is more common to begin by **adding a constant** to all values, producing a set of non-negative data to which any power transformation can be applied.

https://en.wikipedia.org/wiki/Power_transform

Box-Cox Transformations (1/3)

$$y(\lambda) = \begin{cases} \dfrac{y^{\lambda}-1}{\lambda}, & \text{if } \lambda \neq 0; \\ \log y, & \text{if } \lambda = 0. \end{cases}$$

Box and Cox(1964)

$$y(\boldsymbol{\lambda}) = \begin{cases} \dfrac{(y+\lambda_2)^{\lambda_1}-1}{\lambda_1}, & \text{if } \lambda_1 \neq 0; \\ \log(y+\lambda_2), & \text{if } \lambda_1 = 0. \end{cases}$$

$\boldsymbol{\lambda} = (\lambda_1, \lambda_2)'$

choose λ_2 such that $y + \lambda_2 > 0$ for any y.

- The aim of the Box-Cox transformations is to ensure the usual assumptions for Linear Model hold.

$$\boldsymbol{y} \sim \mathrm{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I}_n)$$

- Clearly not all data could be power-transformed to Normal. Draper and Cox (1969) studied this problem and conclude that even in cases that no power-transformation could bring the distribution to exactly normal, the usual estimates of lambda will lead to a distribution that satisfies certain restrictions on the first 4 moments, thus will be usually **symmetric**.

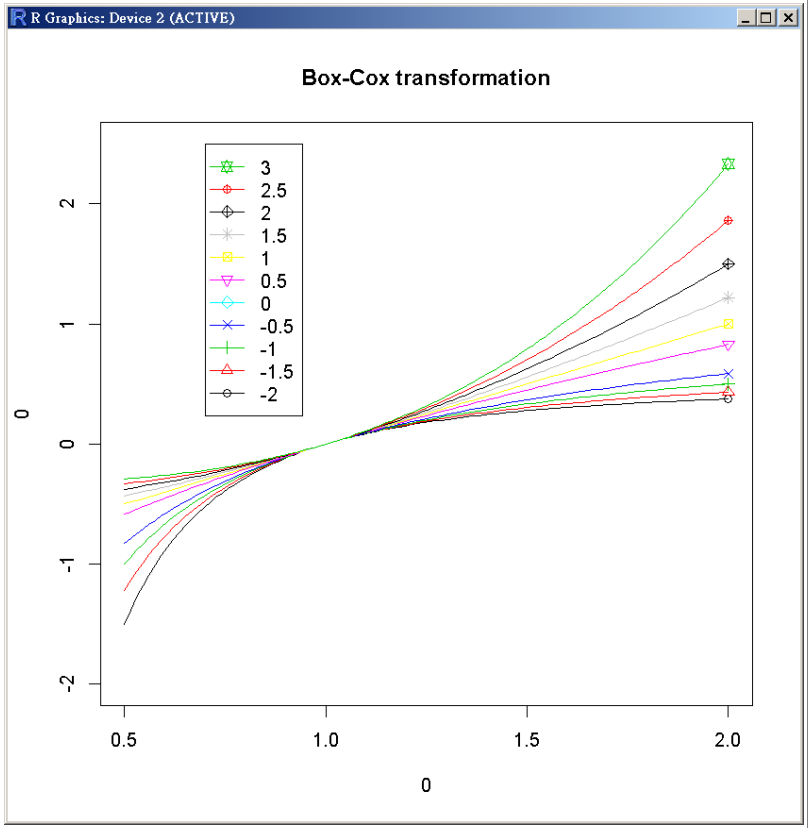
Source: Box-Cox Transformations: An Overview, Pengfei Li, Department of Statistics, University of Connecticut, Apr 11, 2005

Box-Cox Transformations (2/3)

$$x'_\lambda = \frac{e^{\lambda \log(x)} - 1}{\lambda} \approx \frac{\left(1 + \lambda \log(x) + \frac{1}{2}\lambda^2 \log(x)^2 + \cdots\right) - 1}{\lambda} \to \log(x)$$

as $\lambda \to 0$.

```
x <- seq(0.5, 2, length.out=100)
bc <- function(y, lambda){
    (y^lambda -1)/lambda
}
lambda <- seq(-2, 3, 0.5)
plot(0, 0, type="n", xlim=c(0.5, 2),
     ylim=c(-2, 2.5), main="Box-Cox transformation")
for(i in 1:length(lambda)){
   points(x, bc(x, lambda[i]), type="l", col=i)
   points(2, bc(2, lambda[i]), col=i, pch=i)
}
legend(0.7, 2.5, legend=as.character(rev(lambda)),
       lty=1, pch=length(lambda):1,
       col=length(lambda):1)
```

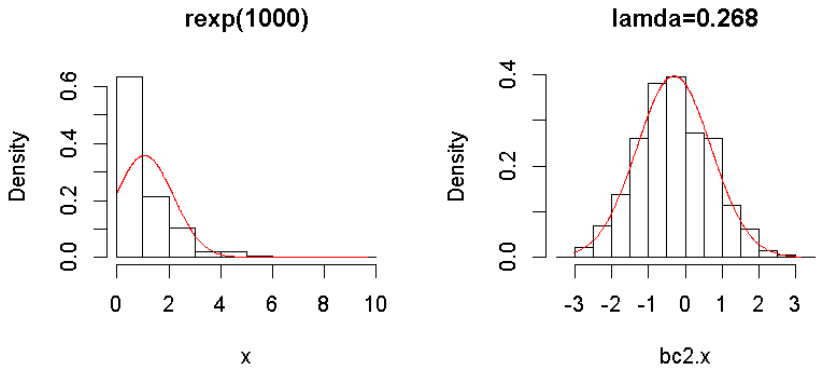


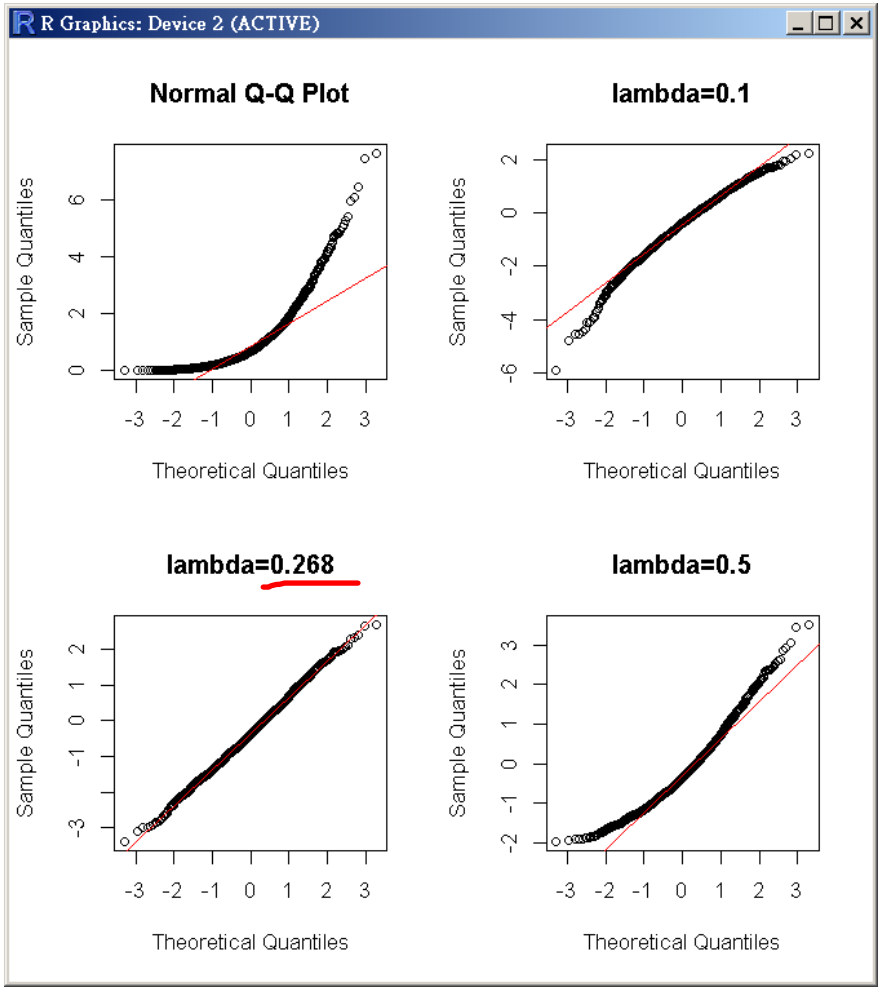
lambda = 0 ?

http://onlinestatbook.com/2/transformations/box-cox.html

Box-Cox Transformations (3/3)

```
> x <- rexp(1000)
> bc <- function(y, lambda){
+     (y^lambda -1)/lambda
+ }
> bc1.x <- bc(x, 0.1)
> bc2.x <- bc(x, 0.268)
> bc3.x <- bc(x, 0.5)
> par(mfrow=c(2, 2))
> qqnorm(x); qqline(x, col="red")
> qqnorm(bc1.x, main="lambda=0.1")
> qqline(bc1.x, col="red")
> qqnorm(bc2.x, main="lambda=0.268")
> qqline(bc2.x, col="red")
> qqnorm(bc3.x, main="lambda=0.5")
> qqline(bc3.x, col="red")
```





$$\left(\Phi^{-1}\left(\frac{i-0.5}{n}\right), x_{(i)}\right), \qquad \text{for } i = 1, 2, \ldots, n,$$

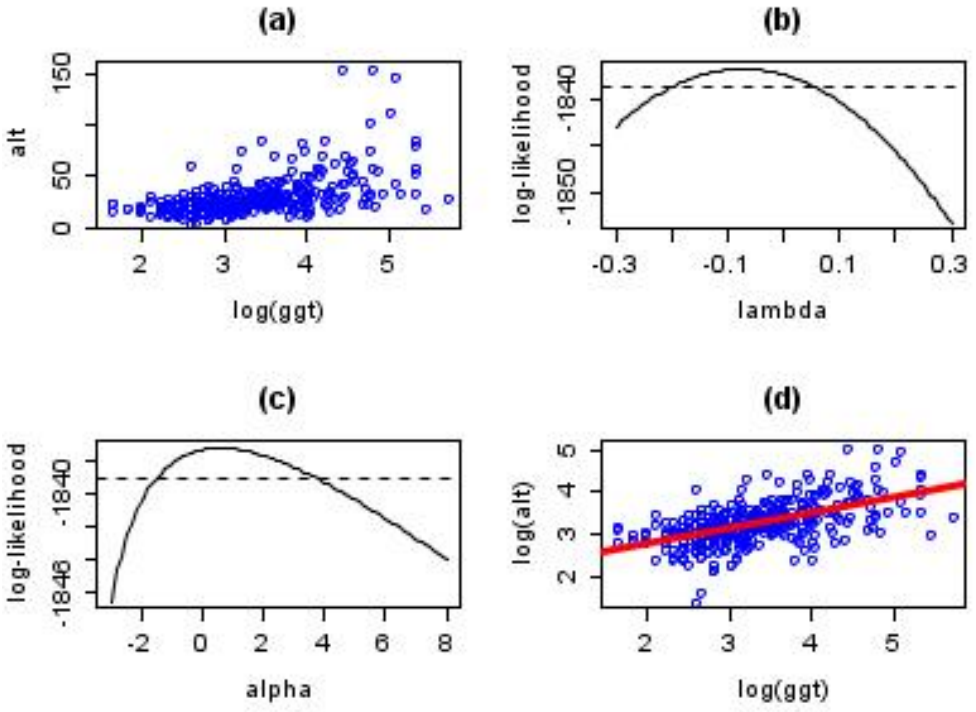
Source: Box-Cox Transformations: An Overview, Pengfei Li, Department of Statistics, University of Connecticut, Apr 11, 2005

範例: BUPA Liver Data Set

- The BUPA liver data set contains data on liver enzymes ALT and γGT. Suppose we are interested in using **log(γGT)** to predict **ALT**. (a): there appears to be non-constant variance, and a Box–Cox transformation might help.
- Possibly, the transformation could be improved by adding a shift parameter to the log transformation. (c): in this case, the maximum of the likelihood is close to zero suggesting that a shift parameter is not needed.

- (d) The final panel shows the transformed data with a superimposed regression line.
- Note that although Box–Cox transformations can make big improvements in model fit, there are some issues that the transformation cannot help with. In the current example, the data are rather heavy-tailed so that the assumption of normality is not realistic and a robust regression approach leads to a more precise model.

https://en.wikipedia.org/wiki/Power_transform



Box-Cox Transformations: Summary

- It is not always necessary or desirable to transform a data set to resemble a normal distribution. However, if symmetry or normality are desired, they can often be induced through one of the power transformations.

$$y(\lambda) = \begin{cases} \frac{y^{\lambda}-1}{\lambda}, & \text{if } \lambda \neq 0; \\ \log y, & \text{if } \lambda = 0. \end{cases}$$

λ = 1.00: no transformation needed; produces results identical to original data

λ = 0.50: square root transformation

λ = 0.33: cube root transformation

λ = 0.25: fourth root transformation

λ = 0.00: natural log transformation

λ = -0.50: reciprocal square root transformation

λ = -1.00: reciprocal (inverse) transformation

and so forth.

Modified Box-Cox Transformations

Manly(1971)

$$y(\lambda) = \begin{cases} \frac{e^{\lambda y}-1}{\lambda}, & \text{if } \lambda \neq 0; \\ y, & \text{if } \lambda = 0. \end{cases}$$

Negative y's could be allowed. The transformation was reported to be successful in transform unimodal skewed distribution into normal distribution, but is not quite useful for **bimodal** or **U-shaped distribution**.

John and Draper(1980) "Modulus Transformation"

$$y(\lambda) = \begin{cases} \text{Sign}(y)\frac{(|y|+1)^{\lambda}-1}{\lambda}, & \text{if } \lambda \neq 0; \\ \text{Sign}(y)\log(|y|+1), & \text{if } \lambda = 0, \end{cases}$$

$$\text{Sign}(y) = \begin{cases} 1, & \text{if } y \geq 0; \\ -1, & \text{if } y < 0. \end{cases}$$

Bickel and Doksum(1981)

$$y(\lambda) = \frac{|y|^{\lambda}\text{Sign}(y)-1}{\lambda}, \quad \text{for } \lambda > 0,$$

Yeo and Johnson(2000)

$$y(\lambda) = \begin{cases} \frac{(y+1)^{\lambda}-1}{\lambda}, & \text{if } \lambda \neq 0,\ y \geq 0; \\ \log(y+1), & \text{if } \lambda = 0,\ y \geq 0; \\ \frac{(1-y)^{2-\lambda}-1}{\lambda-2}, & \text{if } \lambda \neq 2,\ y < 0; \\ -\log(1-y), & \text{if } \lambda = 2,\ y < 0. \end{cases}$$

Source: Box-Cox Transformations: An Overview, Pengfei Li, Department of Statistics, University of Connecticut, Apr 11, 2005

Transformations for Proportions and Percents: Logit Transformation (2/2)

- If values are naturally restricted to be in the range 0 to 1, not including the end-points, then a logit transformation may be appropriate: this yields values in the range (−∞,∞).

- The logit of a number p between 0 and 1 is given by the formula:

$$\operatorname{logit}(p) = \log\left(\frac{p}{1-p}\right) = \log(p) - \log(1-p) = -\log\left(\frac{1}{p} - 1\right).$$

- When the function's parameter represents a probability p, the logit function gives the log-odds, or the logarithm of the odds p/(1 − p).

$$P(y_i = 0) = 1 - \pi_i, \;\; P(y_i = 1) = \pi_i$$

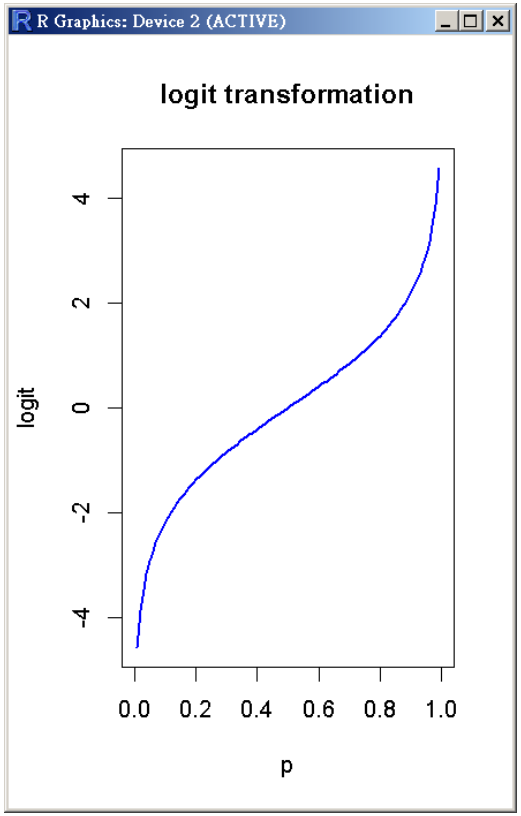
$$\text{Logistic link function: } g(\pi) = \log(\frac{\pi}{1-\pi})$$

$$\text{Logistic regression: } \log(\frac{\pi}{1-\pi}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

Transformations for Proportions and Percents: Logit Transformation (2/2)

- This transformation treats very small and very large values symmetrically, pulling out the tails and pulling in the middle around 0.5 or 50%. The plot of p against $logit(p)$ is thus a flattened S-shape.

- Strictly, *logit p* cannot be determined for the extreme values of 0 and 1 (100%): if they occur in data, there needs to be some adjustment.



Variance Stabilizing Transformations

- Many types of statistical data exhibit a "**variance-on-mean relationship**", meaning that the variability is different for data values with different expected values.

- A variance-stabilizing transformation aims to remove a variance-on-mean relationship, so that the variance becomes **constant** relative to the mean.

- Examples of variance-stabilizing transformations
  - Fisher transformation for the sample correlation coefficient,
  - Square root transformation or Anscombe transform for Poisson data (count data),
  - Box-Cox transformation for regression analysis and
  - Arcsine square root transformation or angular transformation for proportions (binomial data).

https://en.wikipedia.org/wiki/Data_transformation_%28statistics%29

Standardization (1/5)

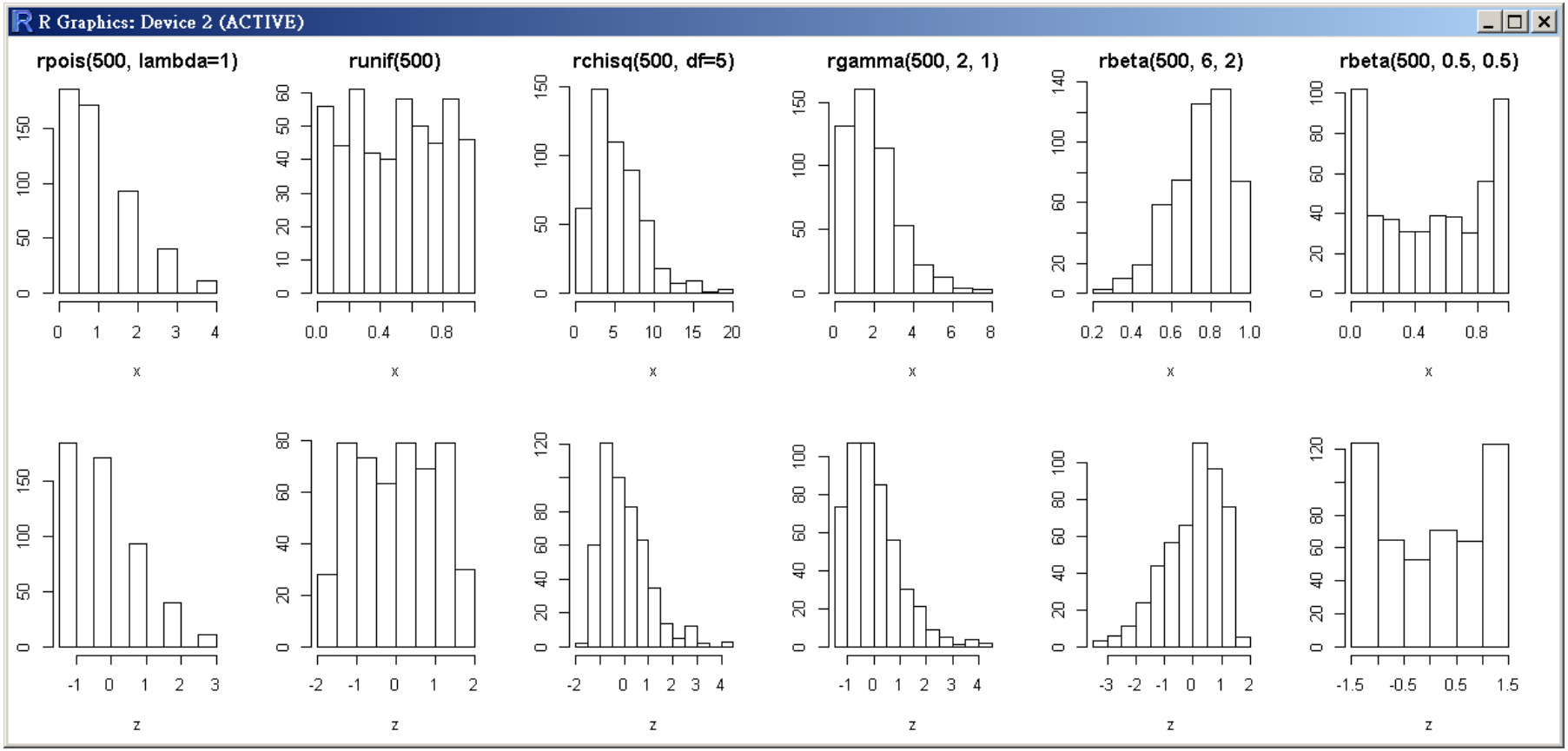
- Standardization, $z = (x\text{-}x.bar)/s$, (called z-score): the new variate z will have a mean of zero and a variance of one. (also called centering and scaling.)

- If the variables are measurements along a **different scale** or if the standard deviations for the variables are different from one another, then one variable might **dominate** the distance (or some other similar calculation) used in the analysis:
- Standardization is useful for comparing variables expressed in different units.

- In some multivariate contexts, the transformations may be applied to each variable separately.
  - **Standardization makes no difference to the shape of a distribution**.

Standardization (2/5)

- Standardization makes no difference to the shape of a distribution.




```
x <- rpois(500, lambda=1)
hist(x, main="rpois(500, lambda=1)"); z <- scale(x); hist(z, main="")
```

Standardization (3/5)

In Clustering Analysis

- When the z-score transformation is used in a clustering context, it is important that it be applied in a global manner across all observations.
- If standardization is done within clusters, then false and misleading clustering solutions can result [Milligan and Cooper, 1988].

In Calculating Distance/Similarity (e.g., multidimensional scaling)

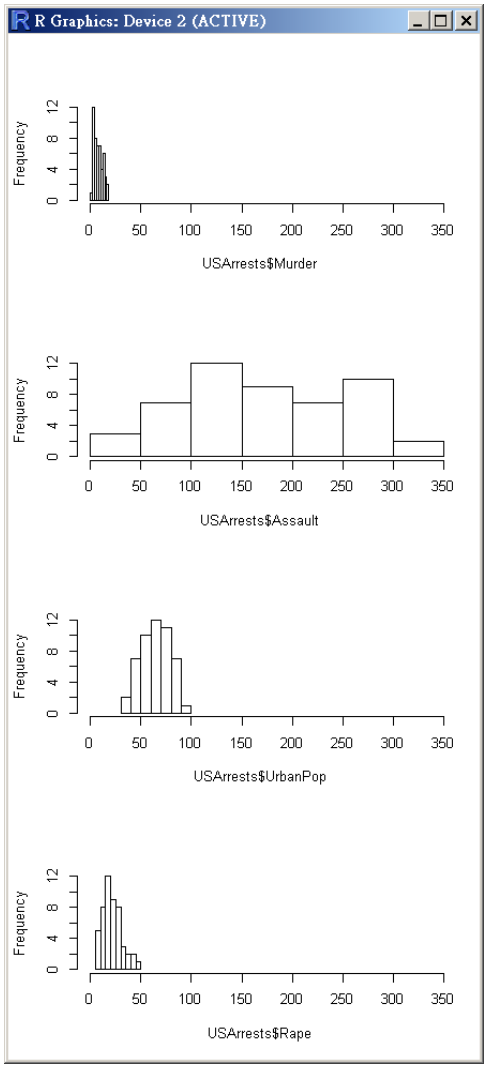
- Euclidean distances calculated on data that have been transformed using the two formulas result in identical dissimilarity values.
- For robust versions of Equations, we can substitute the **median** and the **interquartile range** for the sample mean and sample variance.

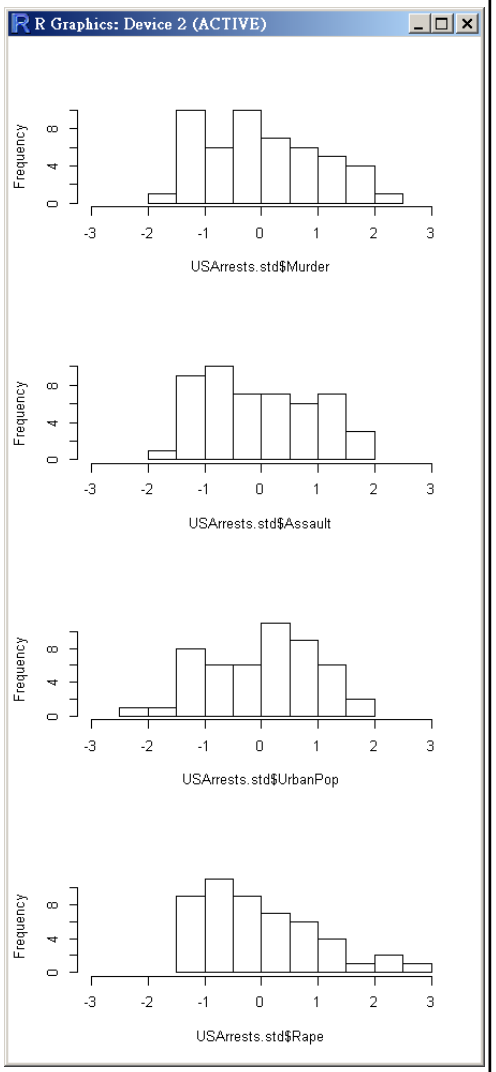
Standardization (4/5)

USArrests {datasets}: Violent Crime Rates by US State
A data frame with 50 observations on 4 variables.
[1] Murder: Murder arrests (per 100,000)
[2] Assault: Assault arrests (per 100,000)
[3] UrbanPop: Percent urban population
[4] Rape: Rape arrests (per 100,000)

```
> head(USArrests)
           Murder Assault UrbanPop Rape
Alabama      13.2     236       58 21.2
Alaska       10.0     263       48 44.5
Arizona       8.1     294       80 31.0
Arkansas      8.8     190       50 19.5
California    9.0     276       91 40.6
Colorado      7.9     204       78 38.7
> par(mfrow=c(4,1))
> r <- range(USArrests)
> hist(USArrests$Murder, xlim = r)
> hist(USArrests$Assault, xlim = r)
> hist(USArrests$UrbanPop, xlim = r)
> hist(USArrests$Rape, xlim = r)

> USArrests.std <- as.data.frame(
apply(USArrests, 2, scale))
> r.std <- c(-3, 3)
> hist(USArrests.std$Murder, xlim = r.std)
> hist(USArrests.std$Assault, xlim = r.std)
> hist(USArrests.std$UrbanPop, xlim = r.std)
> hist(USArrests.std$Rape, xlim = r.std)
```

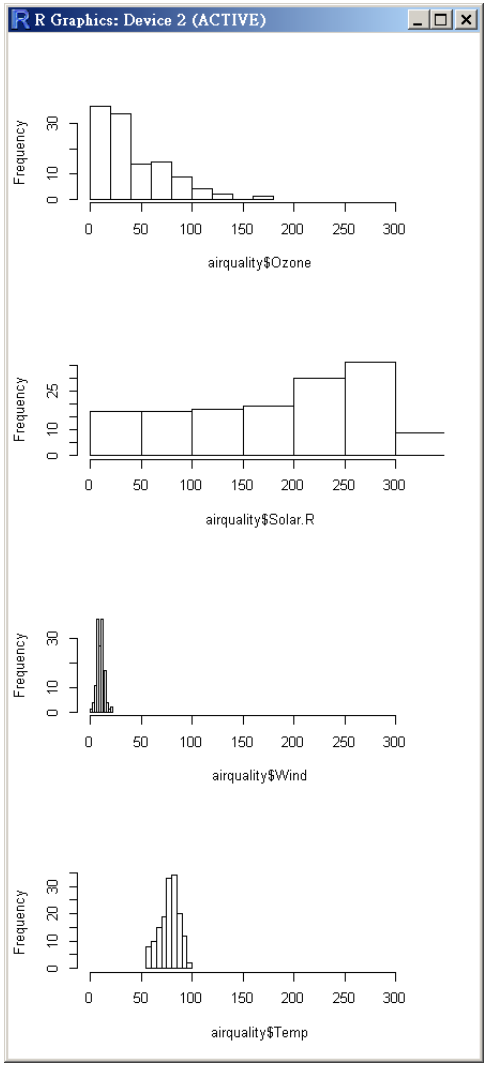


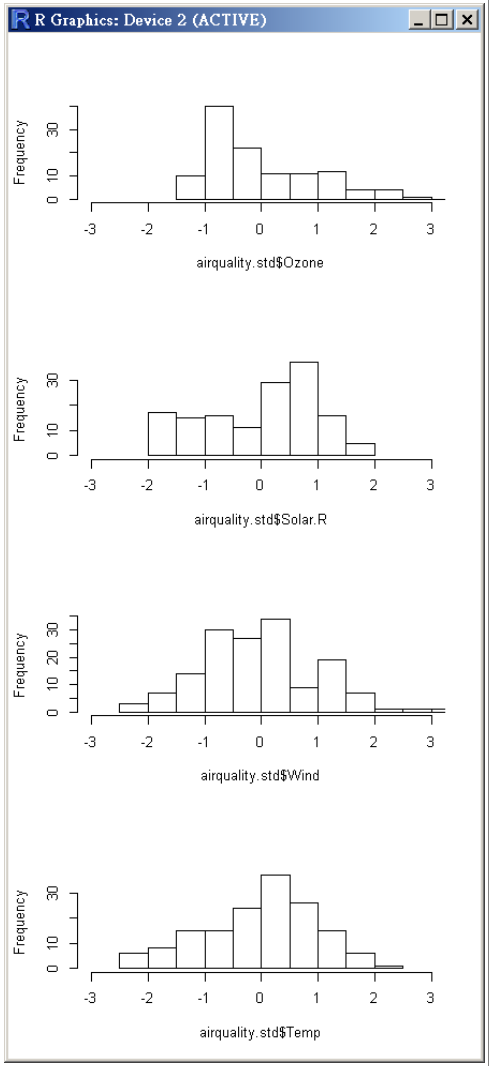


Standardization (5/5)

airquality {datasets}
New York Air Quality Measurements: Daily air quality measurements in New York, May to September 1973.
A data frame with 154 observations on 6 variables.
[1] Ozone: Ozone (ppb)
[2] Solar.R: Solar R (lang)
[3] Wind: Wind (mph)
[4] Temp: Temperature (degrees F)
[5] Month: Month (1--12)
[6] Day: Day of month (1--31)

```
> head(airquality )
  Ozone Solar.R Wind Temp Month Day
1    41     190  7.4   67     5   1
2    36     118  8.0   72     5   2
3    12     149 12.6   74     5   3
4    18     313 11.5   62     5   4
5    NA      NA 14.3   56     5   5
6    28      NA 14.9   66     5   6
> r <- range(airquality[,1:4], na.rm = T)
> hist(airquality$Ozone , xlim = r)
> hist(airquality$Solar.R, xlim = r)
> hist(airquality$Wind, xlim = r)
> hist(airquality$Temp, xlim = r)
>
> airquality.std <- as.data.frame(
apply(airquality, 2, scale))
> r.std <- c(-3, 3)
> hist(airquality.std$Ozone, xlim = r.std)
> hist(airquality.std$Solar.R, xlim = r.std)
> hist(airquality.std$Wind, xlim = r.std)
> hist(airquality.std$Temp, xlim = r.std)
```





範例: Microarray Data of Yeast Cell Cycle

- The data consists of several sub-sets collected under different conditions: alpha factor arrest, elutriation, arrest of cdc15 and cdc28 temperature-sensitive mutant.
- Each of these sub-sets is a single experiment. These experiment methods are used to synchronize the yeast cell cycle. Synchronized by alpha factor arrest method: Spellman et al. (1999).
- Time course data: every 7 minutes and totally 18 time points.
- Known genes: there are 103 cell cycle-regulated genes by traditional method in G1, S, S/G2, G2/M, or M/G1.

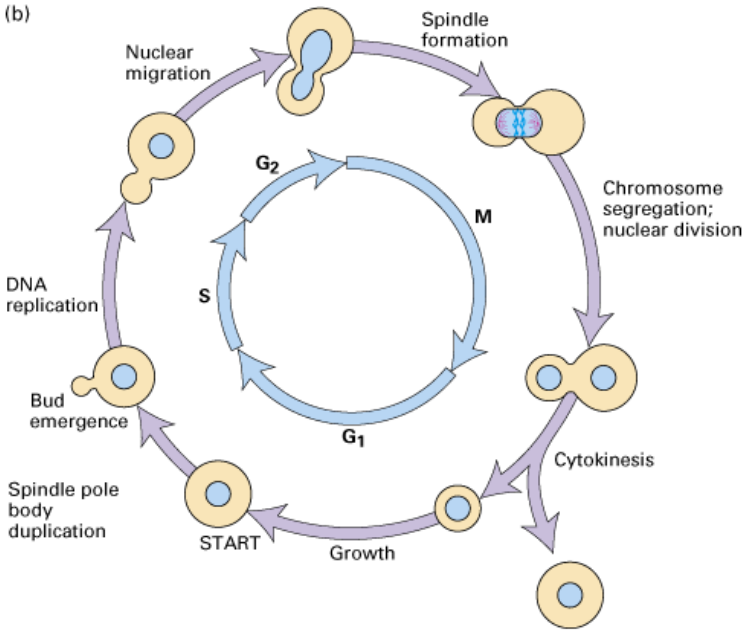


Image: http://www.pha.jhu.edu/~ghzheng/old/webct/note7_3.htm

Microarray Data of Yeast Cell Cycle.xls

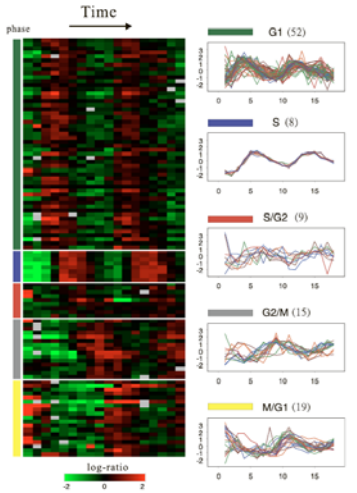
	A	B	C	D	E	F	G	H
1	gene	phase.name	alpha0	alpha7	alpha14	alpha21	alpha28	alpha35
2	YAR007C	G1	-0.48	-0.42	0.87	0.92	0.67	-0.18
3	YBL035C	G1	-0.39	-0.58	1.08	1.21	0.52	-0.33
4	YBR023C	G1	0.87	0.25	-0.17	0.18	-0.13	-0.44
5	YBR067C	G1	1.57	1.03	1.22	0.31	0.16	-0.49
6	YBR088C	G1	-1.15	-0.86	1.21	1.62	1.12	0.16
7	YBR278W	G1	0.04	-0.12	0.31	0.16	0.17	-0.06
8	YCL055W	G1	2.95	0.45	-0.40	-0.66	-0.59	-0.38
9	YDL003W	G1	-1.22	-0.74	1.34	1.50	0.63	0.29
10	YDL055C	G1	-0.73	-1.06	-0.79	-0.02	0.16	0.44
11	YDL102W	G1	-0.58	-0.40	0.13	0.58	-0.09	0.02
12	YDL164C	G1	-0.50	-0.42	0.66	1.05	0.68	0.06
13	YDL197C	G1	-0.86	-0.29	0.42	0.46	0.30	0.10
14	YDL227C	G1	-0.16	0.29	0.17	-0.28	-0.02	-0.55
15	YDR052C	G1	-0.36	-0.03	-0.03	-0.08	-0.23	-0.25
16	YDR097C	G1	-0.72	-0.85	0.54	1.04	0.84	0.24
17	YDR113C	G1	-0.78	-0.52	0.26	0.20	0.48	0.48
18	YDR309C	G1	0.60	-0.55	0.41	0.45	0.18	-0.66
19	YDR356W	G1	-0.20	-0.67	0.13	0.10	0.38	0.44
20	YER001W	G1	-2.29	-0.64	0.77	1.60	0.53	0.55
21	YER070W	G1	-1.46	-0.76	1.08	1.50	0.74	0.47
22	YER095W	G1	-0.57	0.42	1.03	1.35	0.64	0.42
23	YGL163C	G1	-0.11	0.13	0.41	0.60	0.23	0.31
24	YGL225W	G1	-1.08	-0.99	-0.16	0.20	0.61	0.37
25	YGR109C	G1	-1.79	0.94	2.13	1.75	0.23	0.15

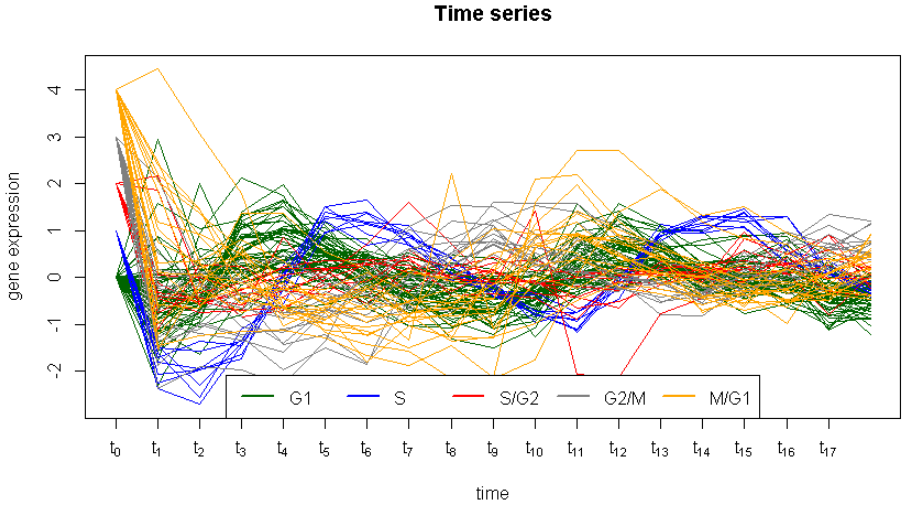
LogRatio

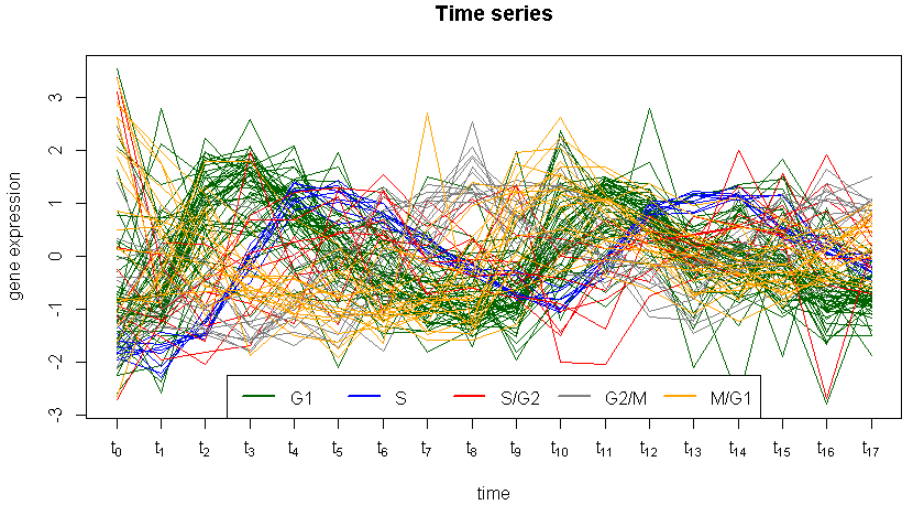
Spellman et al., (1998). Comprehensive Identification of Cell Cycle-regulated Genes of the Yeast Saccharomyces cerevisiae by Microarray Hybridization. Molecular Biology of the Cell 9, 3273-3297.

Standardization in Time Series Microarray Gene Expression Experiments

```
cell.raw <- read.table("trad_alpha103.txt", row.names=1, header=T)
head(cell.raw)
cell.xdata <- t(scale(t(cell.raw[,2:19]), center=T, scale=T))
y.C <-  as.integer(cell.raw[,1])
table(y.C)
no.cluster <- length(unique(y.C))
cellcycle.color <- c("darkgreen", "blue", "red", "gray50", "orange")
p <- ncol(cell.raw) -1
ycolors <- cellcycle.color[y.C+1]
my.pch <- c(1:no.cluster)[y.C+1]
phase <- c("G1", "S", "S/G2", "G2/M", "M/G1")
matplot(t(cell.xdata), pch = 1:p, lty=1, type = "l", ylab="gene expression",
            col=ycolors, xlab="time", main="Time series", xaxt="n")
time.label <- parse(text=paste("t[",0:p,"]",sep=""))
axis(1, 1:(p+1), time.label)
legend("bottom", legend=phase, col=cellcycle.color, lty=1, horiz = T, lwd=2)
```





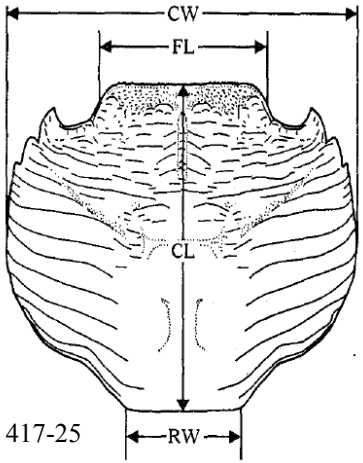


The data map for 103 cell cycle-regulated genes and the plots of time courses for each phase. Each expression profile is normalized as mean equals zero and variance 1.

範例: Crab Data (1/4)

crabs {MASS}
Morphological Measurements on Leptograpsus Crabs
Description: The crabs data frame has 200 rows and 8 columns, describing 5 morphological measurements on 50 crabs each of two colour forms and both sexes, of the species Leptograpsus variegatus (紫岩蟹) collected at Fremantle, W. Australia.

This data frame contains the following columns:
sp: species - "B" or "O" for blue or orange.
sex: “M” or “F” for male or female
index: 1:50 within each of the four groups.
FL: carapace frontal lobe (lip) size (mm).
RW: carapace rear width (mm).
CL: carapace length (mm).
CW: carapace width (mm).
BD: body depth (mm).



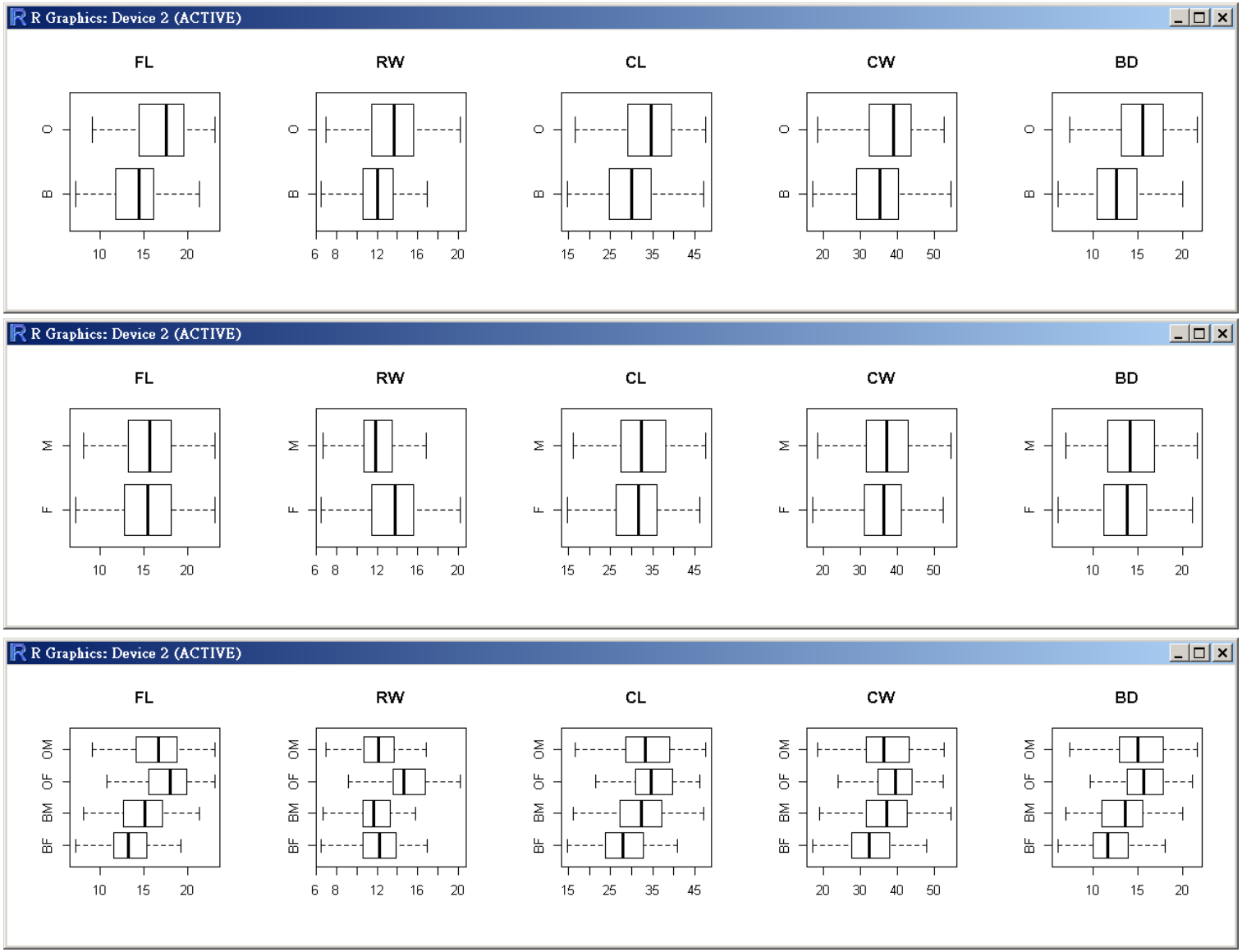
Aust. J. Zool. 1974, 22, 417-25

http://www.qm.qld.gov.au/Find+out+about/Animals+of+Queensland/Crustaceans/Common+marine+crustaceans/Crabs/Purple+Swift-footed+Shore+Crab#.VhPWYiurFhs

```
> library(MASS)
> data(crabs)
```

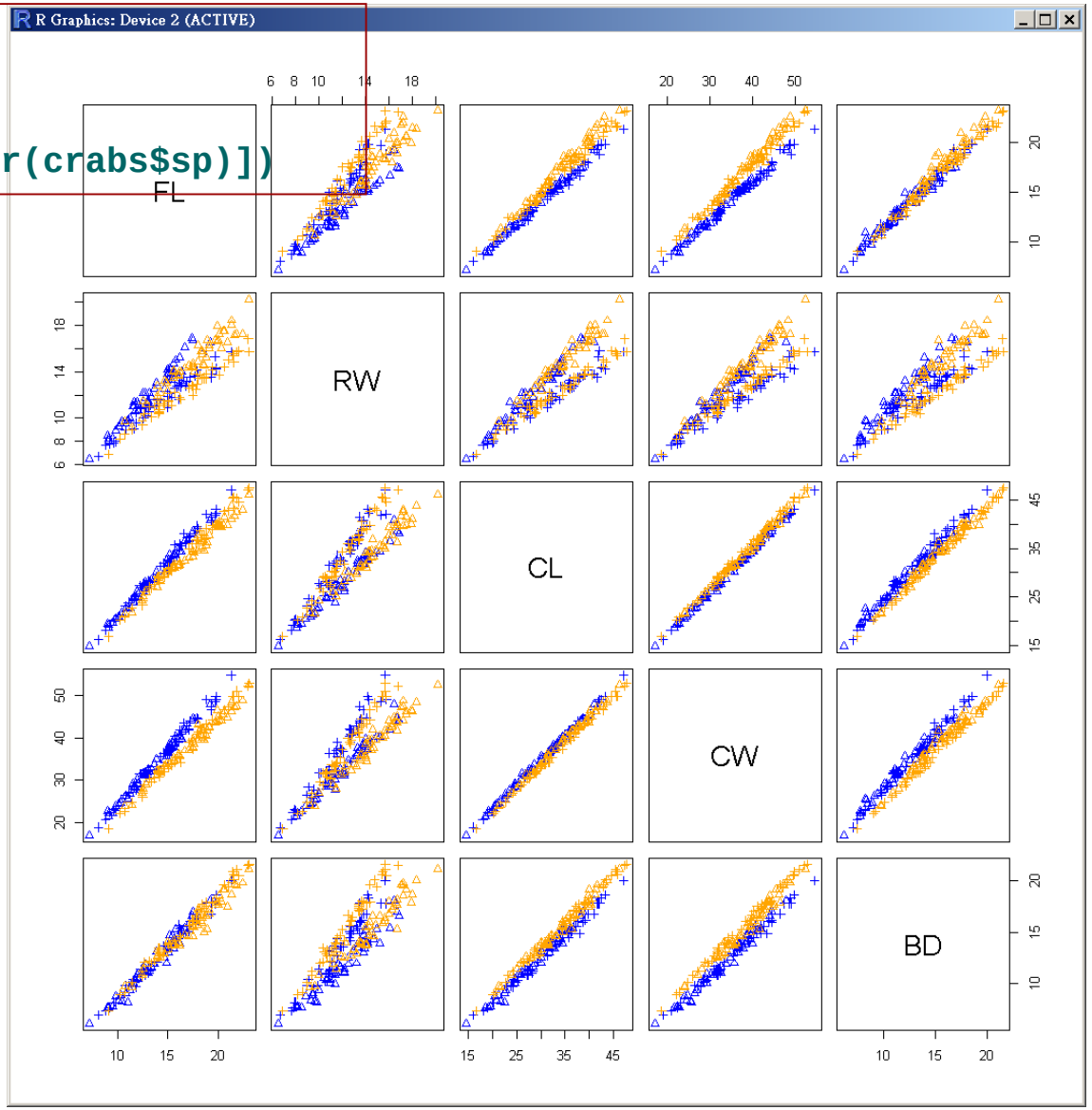
範例: Crab Data (2/4)

```
boxplot(crabs$FL~crabs$sp, main="FL", horizontal=T)
```



範例: Crab Data (3/4)

```
# tri: F,  cross: M
pairs(crabs[,4:8],
pch=as.integer(crabs$sex)+1,
col=c("blue","orange")[as.integer(crabs$sp)])
```



- The analysis of ratios of body measurements is deeply ingrained in the taxonomic literature.
- Whether for plants or animals, certain ratios are commonly indicated in identification keys, diagnoses, and descriptions.

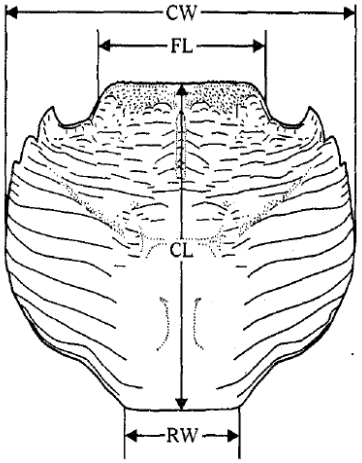
(Hannes Baur and Christoph Leuenberger, Analysis of Ratios in Multivariate Morphometry, Systematic Biology 60(6), 813-825.)

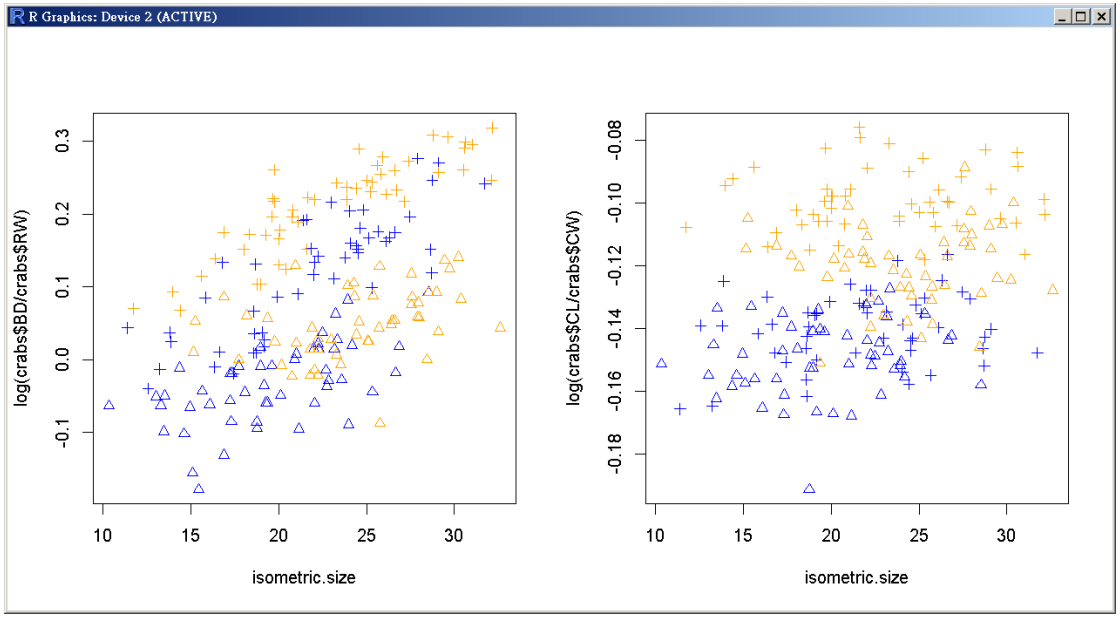
範例: Crab Data (4/4)

- The use of ratios of measurements (i.e., of body proportions), has a long tradition and is deeply ingrained in morphometric taxonomy.

Three size vectors have been commonly proposed in the literature:

(a) isometric size (the arithmetic mean of x),
(b) allometric size,
(c) shape-uncorrelated size.






```
par(mfrow=c(1,2))
mp <- as.integer(crabs$sex)+1
mc <- c("blue","orange")[as.integer(crabs$sp)]
isometric.size <- apply(crabs[,4:8], 1, mean)
plot(isometric.size,  log(crabs$BD/crabs$RW), pch=mp, col=mc)
plot(isometric.size, log(crabs$CL/crabs$CW), pch=mp, col=mc)
```

範例: 房屋實價登錄資料

2014年臺灣資料分析競賽資料 (使用R軟體):
大約 682724筆紀錄，28個變數

	檔案(xls)	縣市別	資料筆數	欄位數
1	List_A	臺北市	54111	28
2	List_B	臺中市	94683	28
3	List_C	基隆市	10833	28
4	List_D	臺南市	54643	28
5	List_E	高雄市	74565	28
6	List_F	新北市	119719	28
7	List_G	宜蘭縣	16104	28
8	List_H	桃園縣	95612	28
9	List_I	嘉義市	6840	28
10	List_J	新竹縣	23399	28
11	List_K	苗栗縣	17515	28
12	List_M	南投縣	13651	28
13	List_N	彰化縣	22613	28
14	List_O	新竹市	15664	28
15	List_P	雲林縣	13171	28
16	List_Q	嘉義縣	9847	28
17	List_T	屏東縣	17583	28
18	List_U	花蓮縣	11327	28
19	List_V	臺東縣	5825	28
20	List_W	金門縣	2509	28
21	List_X	澎湖縣	2423	28
22	List_Z	連江縣	87	28

1	鄉鎮市區	大安區	松山區
2	交易標的	房地(土地+建物)	房地(土地+建物)
3	土地區段位置/建物區段門牌	臺北市大安區和平東路xxx	臺北市松山區三民路xxx
4	土地移轉總面積(平方公尺)	19.39	35.53
5	使用分區或編定	住	住
6	非都市土地使用分區		
7	非都市土地使用地		
8	交易年月	10106	10107
9	交易筆棟數	土地1建物2車位0	土地1建物1車位0
10	移轉層次	五層	七層
11	總樓層數	017	007
12	建物型態	住宅大樓(11層含以上有電梯)	華廈(10層含以下有電梯)
13	主要用途	國民住宅	國民住宅
14	主要建材	鋼筋混凝土造	鋼筋混凝土造
15	建築完成年月	0740522	0810303
16	建物移轉總面積(平方公尺)	100.98	146.66
17	建物現況格局-房	3	3
18	建物現況格局-廳	2	2
19	建物現況格局-衛	1	2
20	建物現況格局-隔間	有	有
21	有無管理組織	有	有
22	總價(元)	18680000	25800000
23	單價(元/平方公尺)	184999	175917
24	車位類別		
25	車位移轉總面積(平方公尺)	0	0
26	車位總價(元)	0	0
27	交易標的橫坐標	305057	306980
28	交易標的縱坐標	2768793	2771975

Species Data Transformation:
The Doubs Fish Data (1/2)

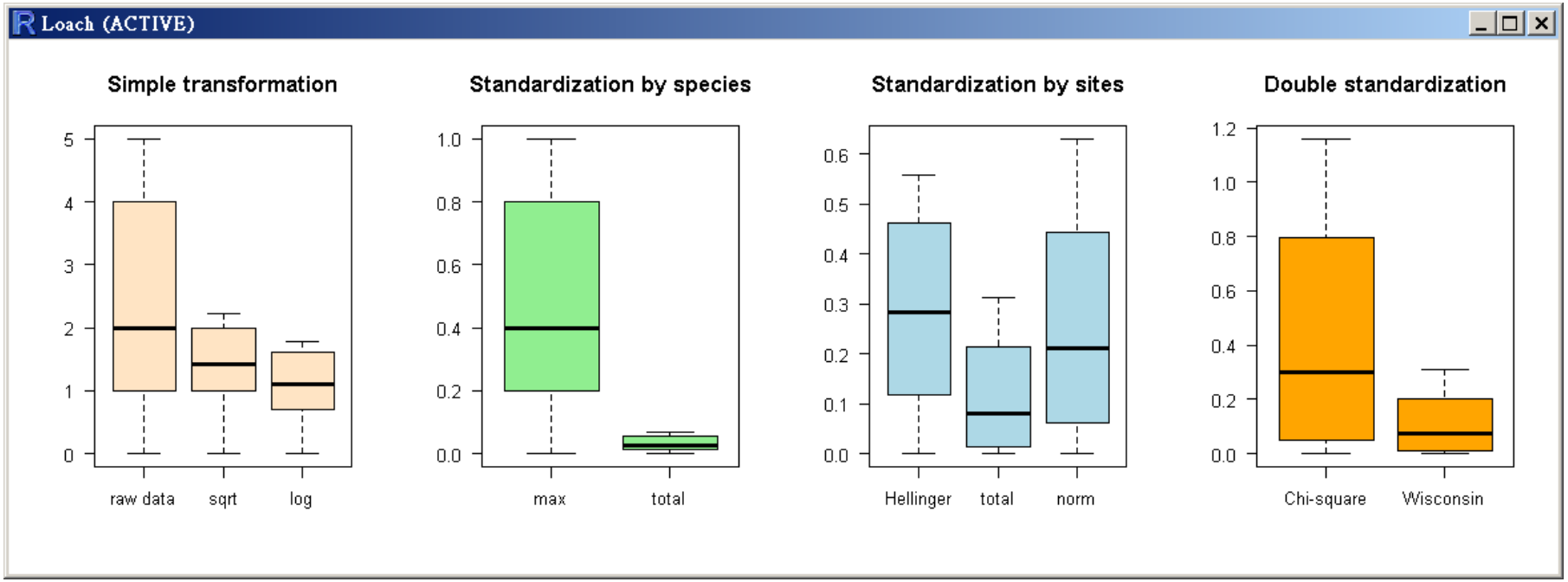
- Species abundances are dimensionally homogenous (expressed in the same physical units), quantitative (count, density, cover, biovolume, biomass, frequency, etc.) or semi-quantitative (classes) variables and restricted to positive or null values (zero meaning absence).

- For these, simple transformations may be used to reduce the importance of observations with very high values:
  - **`sqrt()`** (square root), **`sqrt(sqrt())`** (fourth root), or **`log1p()`** (natural logarithm of abundance + 1 to keep absence as zero).
  - In extreme cases, to give the same weight to all positive abundances irrespective of their values, the data can be transformed to binary 1-0 form (presence–absence).

Species Data Transformation:
The Doubs Fish Data (2/2)

- The decostand( ) function of the vegan package provides many options for common standardization of ecological data.

- Standardization can be done relative to sites (site profiles), species (species profiles), or both (double profiles), depending on the focus of the analysis.



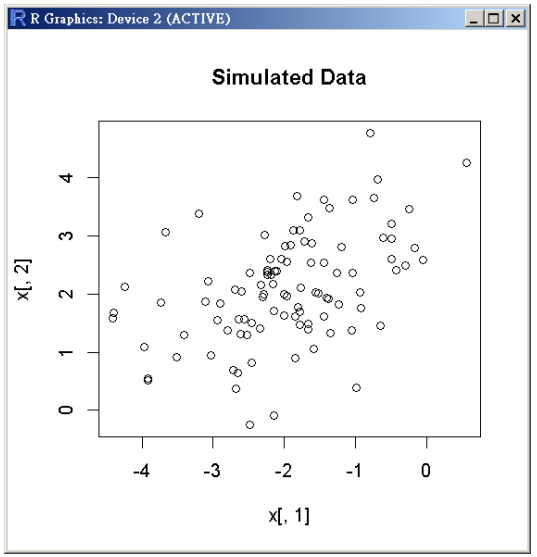
Sphering for Bivariate Variables

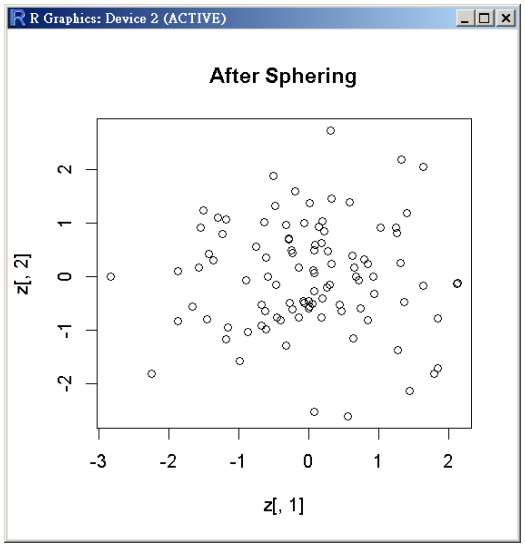
- A scatterplot of the 2-D multivariate normal random variables. Note that these are not centered at the origin, and the cloud is not spherical.

- The sphered data are now centered at the origin with a spherical spread. This is similar to the z-score standardization in 1-D.

```
n <- 100
mu <- c(-2, 2)
sigma <- matrix(c(1, 0.5, 0.5, 1), ncol=2)
library(MASS)
x <- mvrnorm(n, mu, sigma)
plot(x[,1], x[,2], main="Simulated Data")

x.bar <- colMeans(x)
ei <- eigen(cov(x))
D <- diag(ei$values)
V <- ei$vectors
xc <- x - matrix(rep(1, n), ncol=1)%*%x.bar
z <- xc%*%V%*%diag((ei$values)^{-1/2})
plot(z[,1], z[,2], main="After Sphering")
```





Sphering for Multivariate Variables

- The transformed variables will have a p-dimensional mean of 0 and a covariance matrix given by the identity matrix.

Sliced Inverse Regression for Dimension Reduction

KER-CHAU LI*

Journal of the American Statistical Association
June 1991, Vol. 86, No. 414, Theory and Methods

$$y = f(\beta_1 \mathbf{x}, \beta_2 \mathbf{x}, \ldots, \beta_K \mathbf{x}, \epsilon). \qquad (1.1)$$

$$\hat{\Sigma}_{\mathbf{xx}} = \frac{1}{n-1} \sum_{i=1}^{n} \left(\mathbf{x}_i - \bar{\mathbf{x}}\right)\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)^T$$

An $n \times n$ matrix A is diagonalizable if there is a matrix V and a diagonal matrix D such that $A = VDV^{-1}$. This happens if and only if A has n eigenvectors which constitute a basis for $\mathbf{C}^n$. In this case, V can be chosen to be the matrix with the n eigenvectors as columns, and thus a square root of A is

$$R = VSV^{-1},$$

where S is any square root of D.

A in $\mathbf{R}^{nxn}$
- Cholesky Decomposition: $\mathbf{A}=\mathbf{U}^T\mathbf{U}$
- LU Decomposition: $\mathbf{A}=\mathbf{LU}$
- QR Decomposition: $\mathbf{A}=\mathbf{QR}$, **Q**:orthonormal, **R**: upper triangular
- Singular Value Decomposition: $\mathbf{A}=\mathbf{VDV}^T$

4. SLICED INVERSE REGRESSION

A scheme for sliced inverse regression operates on the data $(y_i, \mathbf{x}_i)$ $(i = 1, \ldots, n)$, in the following way:

1. Standardize $\mathbf{x}$ by an affine transformation to get $\tilde{\mathbf{x}}_i = \hat{\Sigma}_{\mathbf{xx}}^{-1/2}(\mathbf{x}_i - \bar{\mathbf{x}})$ $(i = 1, \ldots, n)$, where $\hat{\Sigma}_{\mathbf{xx}}$ and $\bar{\mathbf{x}}$ are the sample covariance matrix and sample mean of $\mathbf{x}$ respectively.
2. Divide range of y into H slices, $I_1, \ldots, I_H$; let the proportion of the y_i that falls in slice h be $\hat{p}_h$; that is $\hat{p}_h = (1/n)\sum_{i=1}^{n} \delta_h(y_i)$, where $\delta_h(y_i)$ takes the values 0 or 1 depending on whether y_i falls into the hth slice I_h or not.
3. Within each slice, compute the sample mean of the $\tilde{\mathbf{x}}_i$'s, denoted by $\hat{m}_h$ $(h = 1, \ldots, H)$, so that $\hat{m}_h = (1/n\hat{p}_h)\sum_{y_i \in I_h} \tilde{x}_i$.
4. Conduct a (weighted) principal component analysis for the data $\hat{m}_h$ $(h = 1, \ldots, H)$ in the following way: Form the weighted covariance matrix $\hat{V} = \sum_{h=1}^{H} \hat{p}_h \hat{m}_h \hat{m}_h'$, then find the eigenvalues and the eigenvectors for $\hat{V}$.
5. Let the K largest eigenvectors (row vectors) be $\hat{\eta}_k$ $(k = 1, \ldots, K)$. Output $\hat{\beta}_k = \hat{\eta}_k \hat{\Sigma}_{\mathbf{xx}}^{-1/2}$ $(k = 1, \ldots, K)$.

Which Transformation? (1/2)

- Use a transformation that other researchers **commonly use in your field**.
- Remember that your data don't have to be perfectly normal and homoscedastic; parametric tests aren't extremely **sensitive** to deviations from their assumptions.
- It is also important that you decide which transformation to use before you do the statistical test. Trying different transformations until you find one that gives you a significant result **is cheating**. (?)
- If you have a **large** number of observations, compare the effects of different transformations on the normality and the homoscedasticity of the variable.
- If you have a **small** number of observations, you may not be able to see much effect of the transformations on the normality and homoscedasticity; in that case, you should use whatever transformation people in your field routinely use for your variable.

http://www.biostathandbook.com/transformation.html

Which Transformation? (2/2)

- The main criterion in choosing a transformation is: **what works with the data?**

It is important to consider as well two questions:

- What makes physical (biological, economic, whatever) sense, for example in terms of limiting behaviour as values get very small or very large? This question often leads to the use of logarithms.

- Can we keep dimensions and units simple and convenient?
  - Prefer measurement scales that are easy to think about.
  - Simplify: The cube root of a volume and the square root of an area both have the dimensions of length. Reciprocals usually have simple units.

Psychological Comments

- Although transformed scales may seem less natural, this is largely a psychological objection. Greater experience with transformation tends to reduce this feeling, simply because transformation **so often works so well**.

- In fact, many familiar measured scales are really transformed scales: decibels (分貝), pH and the Richter scale of earthquake magnitude are all **logarithmic**.

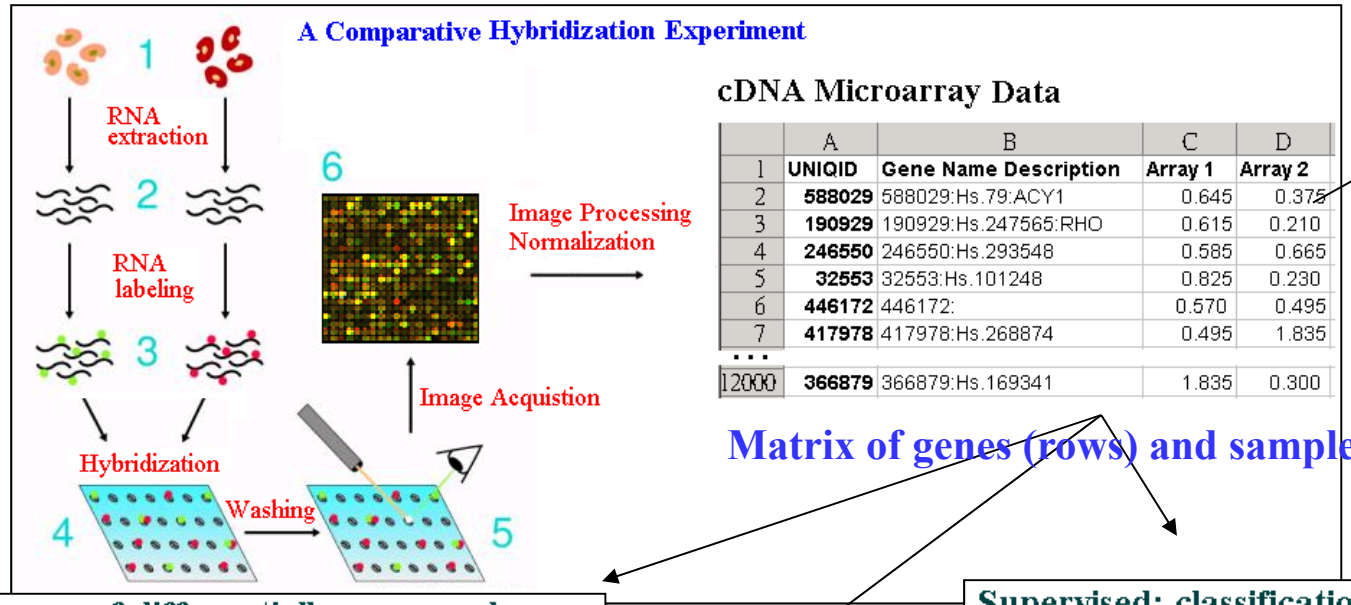
- However, transformations cause debate even among experienced data analysts:
  - "This seems like a kind of cheating. You don't like how the data are, so you decide to change them."
  - "I see that this is a clever trick that works nicely. But how do I know when this trick will work with some other data, or if another trick is needed, or if no transformation is needed?"
  - "Transformations are needed because there is no guarantee that the world works on the scales it happens to be measured on."
  - "Transformations are most appropriate when they match a scientific view of how a variable behaves."
  - Often it helps to transform results back again, using the reverse or inverse transformation.

- **Back transformation:** Even though you've done a statistical test on a transformed variable, such as the log of fish abundance, it is not a good idea to report your means, standard errors, etc. in transformed units.

http://fmwww.bc.edu/repec/bocode/t/transint.html

cDNA Microarray Gene Expression Data

微陣列資料統計分析 Statistical Microarray Data Analysis
http://www.hmwu.idv.tw/index.php/mada



cDNA Microarray Data

	A	B	C	D
1	UNIQID	Gene Name Description	Array 1	Array 2
2	588029	588029:Hs.79:ACY1	0.645	0.375
3	190929	190929:Hs.247565:RHO	0.615	0.210
4	246550	246550:Hs.293548	0.585	0.665
5	32553	32553:Hs.101248	0.825	0.230
6	446172	446172:	0.570	0.495
7	417978	417978:Hs.268874	0.495	1.835
...				
12000	366879	366879:Hs.169341	1.835	0.300

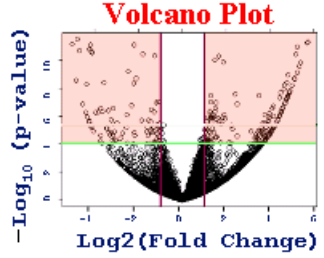
log2(Cy5/Cy3)

Matrix of genes (rows) and samples (columns)

Discovery of differentially expressed genes

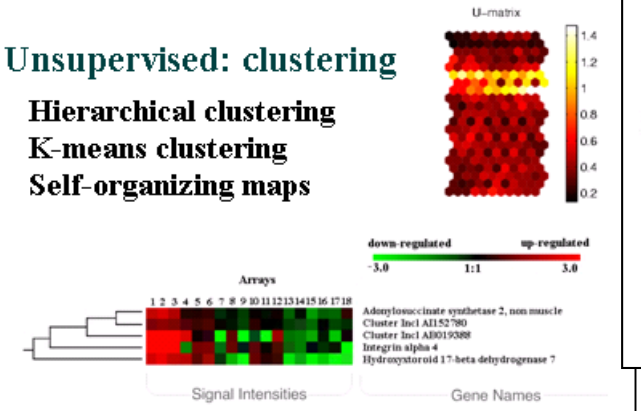
Parametric : t-test
Non-parametric : Wilcoxon, M

Volcano Plot



Unsupervised: clustering

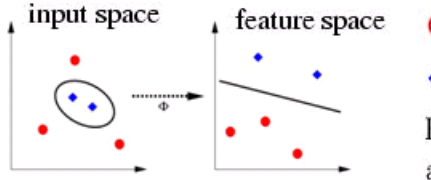
- Hierarchical clustering
- K-means clustering
- Self-organizing maps



Supervised: classification

- Linear discriminants
- Decision trees
- Support vector machines

Support Vector Classifiers



normal
diseased

Boser, Guyon, and Vapnik (1992)

What is Normalization?

- Non-biological factor can contribute to the variability of data, in order to reliably compare data from multiple probe arrays, differences of non-biological origin must be minimized.
- Normalization is a process of reducing unwanted variation across chips.
- It may use information from multiple chips.
  - Normalization corrects for overall chip brightness and other factors that may influence the numerical value of expression intensity,
  - Enabling the user to more confidently compare gene expression estimates between samples.

Why Normalization?

- *Main idea*
  - Remove the systematic bias in the data as completely possible while preserving the variation in the gene expression that occurs because of biologically relevant changes in transcription.
- *Assumption*
  - The average gene does not change in its expression level in the biological sample being tested.
  - Most genes are not differentially expressed or up- and down-regulated genes roughly cancel out the expression effect.

Normalization Methods for cDNA Microarray Data

- **Within-Array Normalization: location**
  - Correcting for Different Responses of the Cy3 and Cy5 Channels
    - Linear Regression of Cy5 Against Cy3 (Global Normalization)
    - Linear Regression of Log Ratio Against Average Intensity
    - Nonlinear Regression of Log Ratio Against Average Intensity (Lowess Normalization)
  - Correcting for Spatial Effects
    - Two-Dimensional Lowess Regression
    - Block-Block Loess Regression (Within Print-tip Group Normalization)
- **Within-Array Normalization: scale**
- **Between-Array Normalization**
  - To enable comparison of multiple arrays
    - Centering, Scaling, Distribution Normalization
- **Paired-slides Normalization**
  (dye swap Experiments) (Slef-normalization)

Case Studies Using R/BioConductor

Statistical Microarray Data Analysis

微陣列資料統計分析

Version: July 01, 2009

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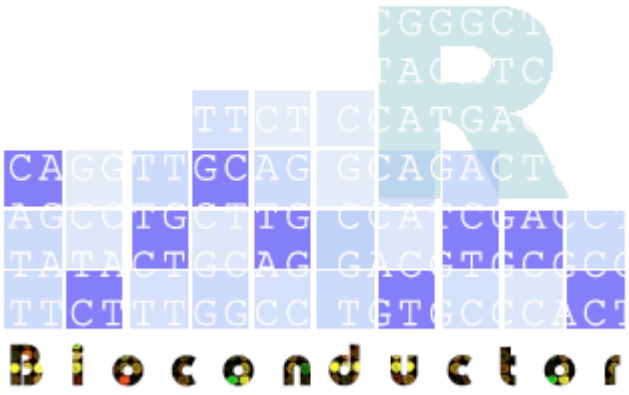

Statistical Microarray Data Analysis

Chapter 2

Preprocessing Two-Color Spotted Microarray

Statistical Microarray Data Analysis

Appendix 2

Lab: Preprocessing of Two-Color Spotted Microarray

Statistical Microarray Data Analysis

Chapter 3

Preprocessing Affymetrix GeneChip Microarray

Statistical Microarray Data Analysis

Appendix 3

Lab: Preprocessing Affymetrix GeneChip Microarray Data