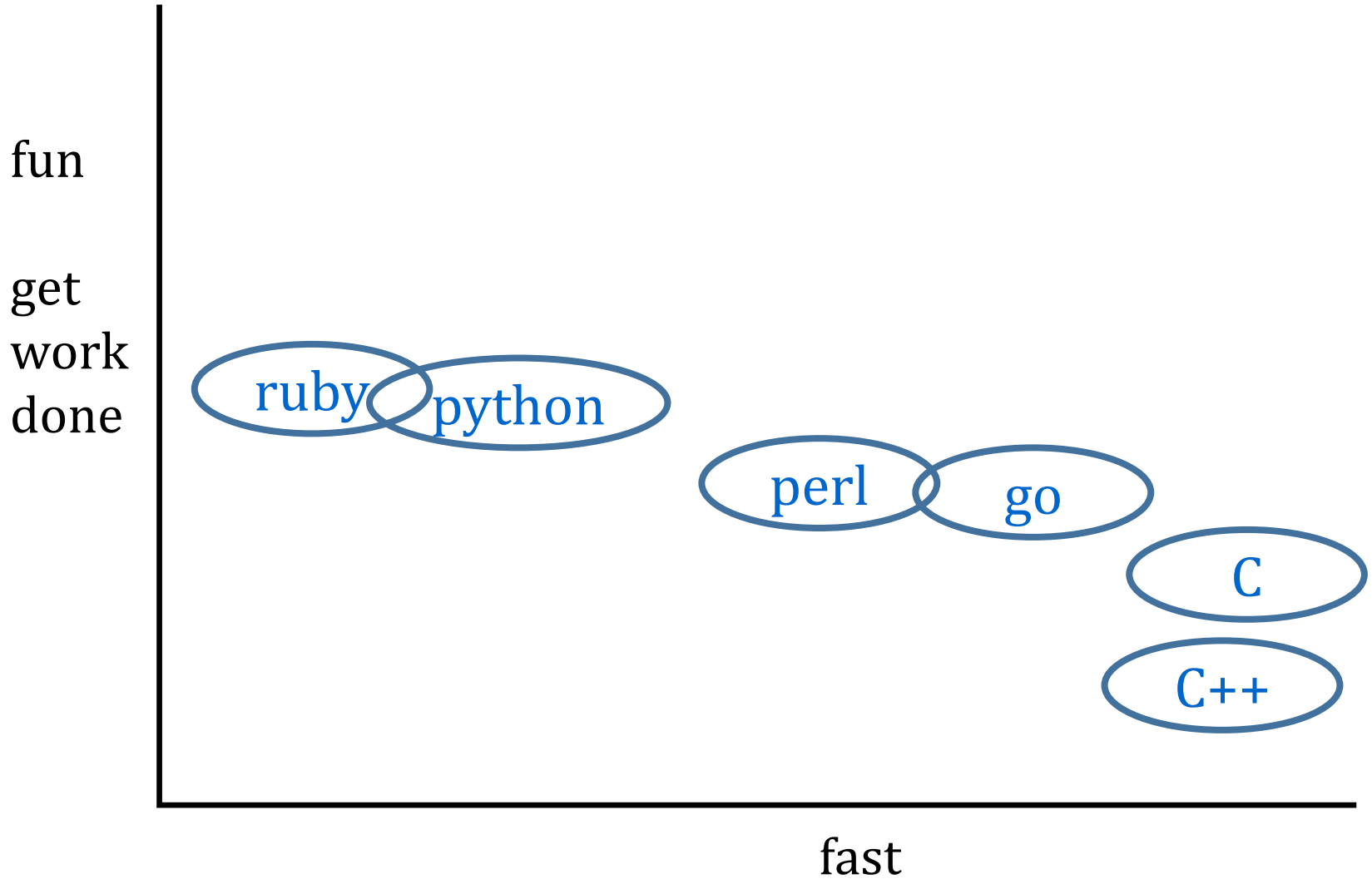
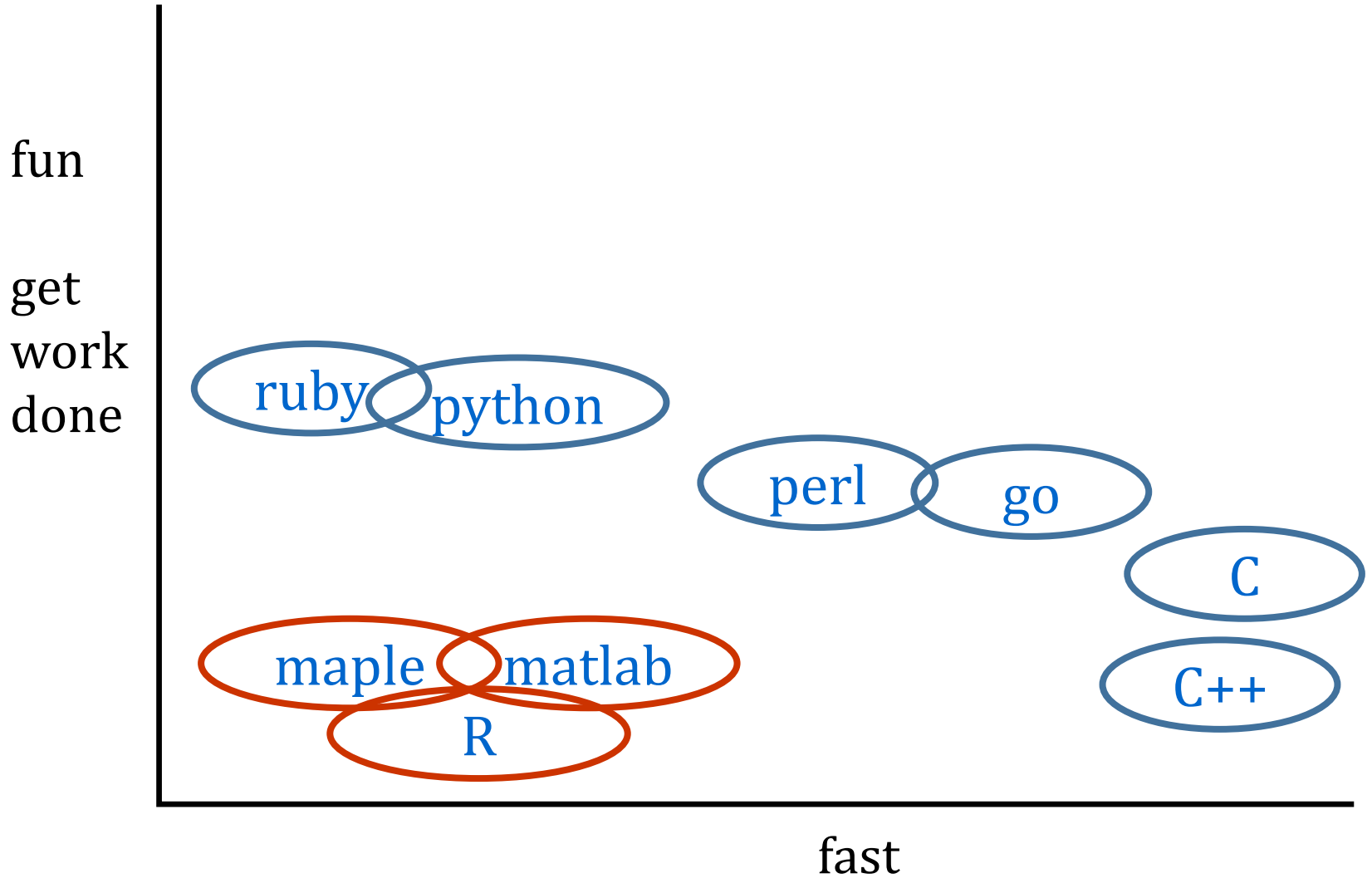
# R and a bit of statistics

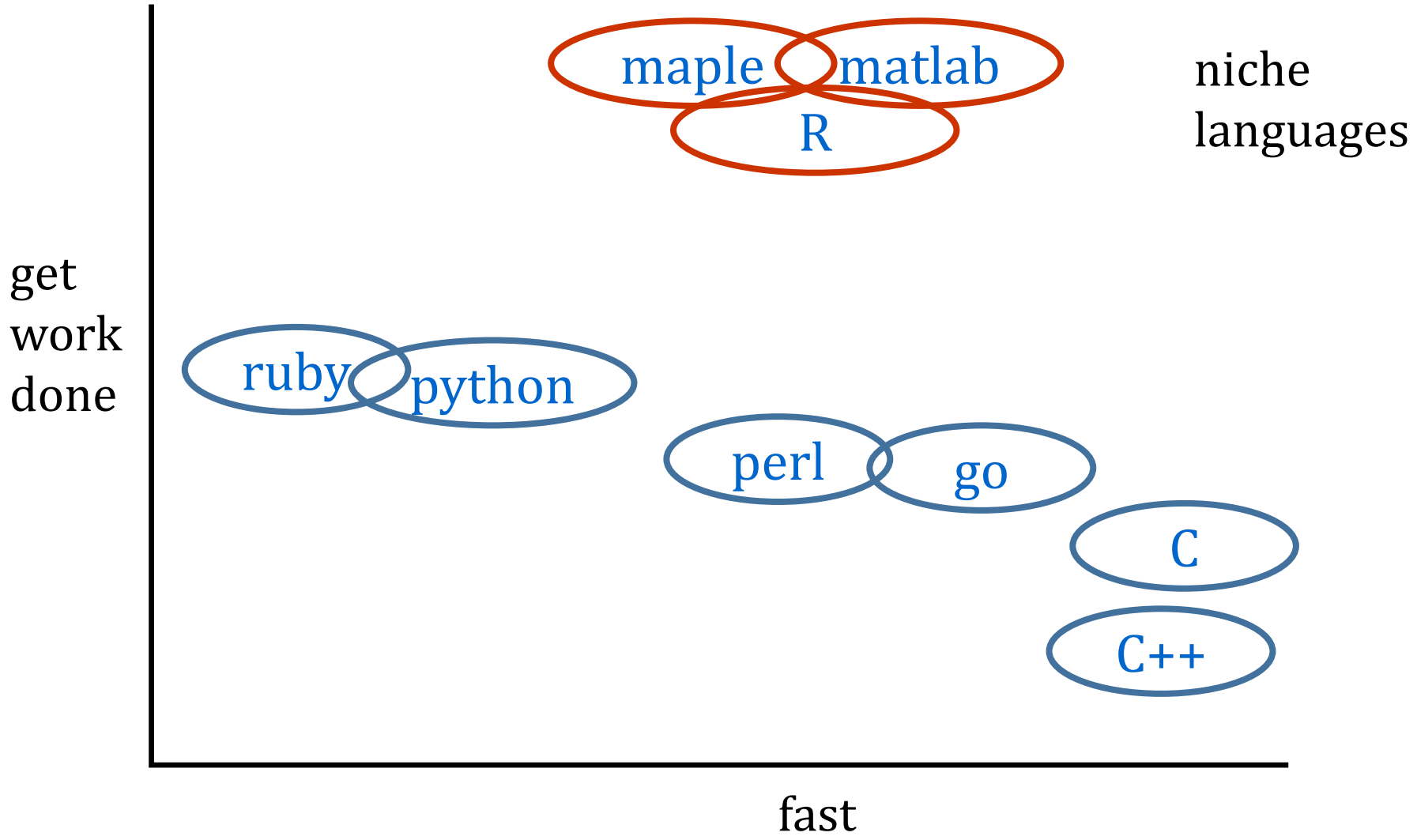
# why ?



# Needleman & Wunsch / parser for mmcif (X-ray) files



# invert matrix, symbolic maths, curve fitting, plotting



# R gives you

- data structures suited to vectors, matrices
  - with appropriate basic operations
- every imaginable distribution
- data fitting
- graphics

Horrible syntax

Starting and stopping

- `R, q()`

Will you get desperate and angry ?

- ask why are there google style guidelines ? a microsoft optimised release ?

# Typical uses

Real data sets

- read, filter, plot, fit, look for correlations…

Playing

- generate a distribution, sample, plot, add noise, ..

# Use

Lots of interfaces

- Rstudio – needs root – good for personal use
- Rcmdr (works on our teaching pool), eclipse
- emacs ESS mode

Code / Scripts / Interactive – not just interpreter

| | | |
|---|---|---|
| C | write, compile, run | compiler |
| Python | write, run | interpreter |
| R | play line by line + write, run | interpreter<br>a bit more .. |

# interpreter, interactive ?

| classic scripting | | no programming |
|---|---|---|
| use an editor / write something | `R` | `Rcmdr, Rstudio` |
| complex | play with command line | Read +display data, like spreadsheet |
| run `Rscript` | | do manipulations from GUI |

# Structural differences

C, C++, python

- cannot add arrays, what does C++ do ? Add ? Concatenate ?
- R: vectors, lists, matrices behave like vectors and matrices

```
> a=c(1, 2, 3)
> b=c(4, 5, 6)
> c=a+b
> c
[1] 5 7 9
```

- do not write `for (i in x) { ...`

# Speed / Memory

Speed

- `a <- b * c` or `x %*% y` or big vectors / matrices – very fast
  - code is recognised, runs hand-crafted routines
- `> for (i in 1:length(a)) { c[i] = a[i] * b[i]}`
  as slow as python

Memory

- like python, perl, ..
  - garbage collected - no memory leaks
  - quite a bit of overhead
- sometimes lots of non-obvious memory – correlations, plots
- easy to make crazy inefficient constructs

# self study

- install.packages('swirl') #download swirl package
- library(swirl) #load in swirl package
  - cheesy, but effective

Essential

**`apropos('etwas')`**

**`?etwas`**

- google R etwas
- Vorsicht – documentation is very formal
- Built-in data sets – often referred to in examples
- **`iris`**, **`mtcars`**, .. type **`data()`**

# Packages

base R = what you get from compiling R distribution

- many popular extensions
- these two lectures – base R

Packages

- $10^5$ R packages on CRAN – good quality control, well supported
  - $10^2$ on our machines `installed.packages()`
- `cran.r-project.org` plotting, advanced statistics, machine learning
- compared to C libraries
  - your matrix implementation is different to mine – try using gsl

Technical…

# Operators

- **`a = 1`** or **`a <- 1`**  R people like **`<-`**
- **`+ - * /`** no surprises – binary operators work on vectors and matrices (element by element – not algebra)
- logical operators
  - >, <, … |, &

Other operations handled by base functions (base = built-in)

- **`mean()`**,**`max()`**, **`median()`**,**`sum()`**,..
  - if you are looking for this kind of common operation
    - look for a built-in – faster than the one you build

# Data Structures

- scalars
- vectors
- matrices
- lists
- data frames

# Scalars

- logical

```
> v <- TRUE
> v
[1] TRUE
> str(v)
 logi TRUE
```

- int
- numeric
- complex
- character

```
> v <- "TRUE" ; v ; str (v)
[1] "TRUE"
chr "TRUE"
```

  - types are automatically chosen

# Vectors

first a little function, **`c()`**

- **`?c`** will tell you what it does **`The default method combines its arguments to form a vector..`**

```
> x <- c(1, 2, 3) ; str (x)
 num [1:3] 1 2 3
```

- indexing from 1 (not zero)
- all elements same type (all float, all int, all logical, ..)

- where do they come from ?
- **`vector()`** ? **`as.vector()`** coming
- data you read in – extract vectors (columns, rows)

# Vectors - Accessing elements

accessing elements..

- **`x[1]`** first element
- **`x[-4]`** everything except fourth element
- **`x[2:4]`**
- **`x[:4]`** elements, 1, 2, 3, 4
- logical versions – compact filtering

```
> x <- c(1, 2, 3, 4, 5) ; x[x>=3]
[1] 3 4 5
```

# matrices

```
m <- matrix(x, nrow = 3, ncol = 4)
```

but more often from

- a data set
- from a calculation like a correlation matrix
- putting vectors together

```
> x <- c(4, 5, 6) ; y <- c(7, 8, 9)
> m <- cbind(x, y) ; m
     x y
[1,] 4 7
[2,] 5 8
[3,] 6 9
> n <- rbind(x, y); n
  [,1] [,2] [,3]
x    4    5    6
y    7    8    9
```

# matrix access

- `m[2, 3]` an element
- `m[, 3]` third column (vector)
- `m[1,]` first row
- logical access – perverse but works

```
x <- c(4, 5, 6) ; y <- c(5, 8, 9)
> m <- cbind(x, y) ; m
     x y
[1,] 4 5
[2,] 5 8
[3,] 6 9
> m[m==5]
[1] 5 5
```

# lists

- not vectors
- mixed types

```
> a <- 'a word'; b <- 1.0; c <- TRUE; d <- c(1, 2, 3)
> l <- list(a, b, c, d) ; str (l)
List of 4
 $ : chr "a word"
 $ : num 1
 $ : logi TRUE
 $ : num [1:3] 1 2 3
```

- group things that are related, but different
- often used for control, functions

# elements in a list

```
> l <- list(x = 1:5, y = c('a', 'b'))  ; l
$x
[1] 1 2 3 4 5
$y                    # There are two things in l, both are vectors
[1] "a" "b"
```

access

```
l[2]
$y
[1] "a" "b"
```

- there are double and single brackets `[]`, `[[]]`

```
> str (l[[1]])
 int [1:5] 1 2 3 4 5   # elements from [[..]]
> str (l[1])
List of 1
 $ x: int [1:5] 1 2 3 4 5 # a new list from [..]
```

# data frames

```
$ cat data.txt
andrew mary
3  4
5  6
7  8
```

- very foreign to C, other languages
  - hash + array ? more generally hash + more general type
- very natural for data

```
> df <- read.table("data.txt", header = TRUE)
> df
  andrew mary
1      3    4
2      5    6
3      7    8
> df$mary
[1] 4 6 8
> str (df$mary)
 int [1:3] 4 6 8    # a vector
```

# data frames

```
$ cat data.txt
andrew mary
3 4
5 6
7 8
```

- If you must, get to rows,

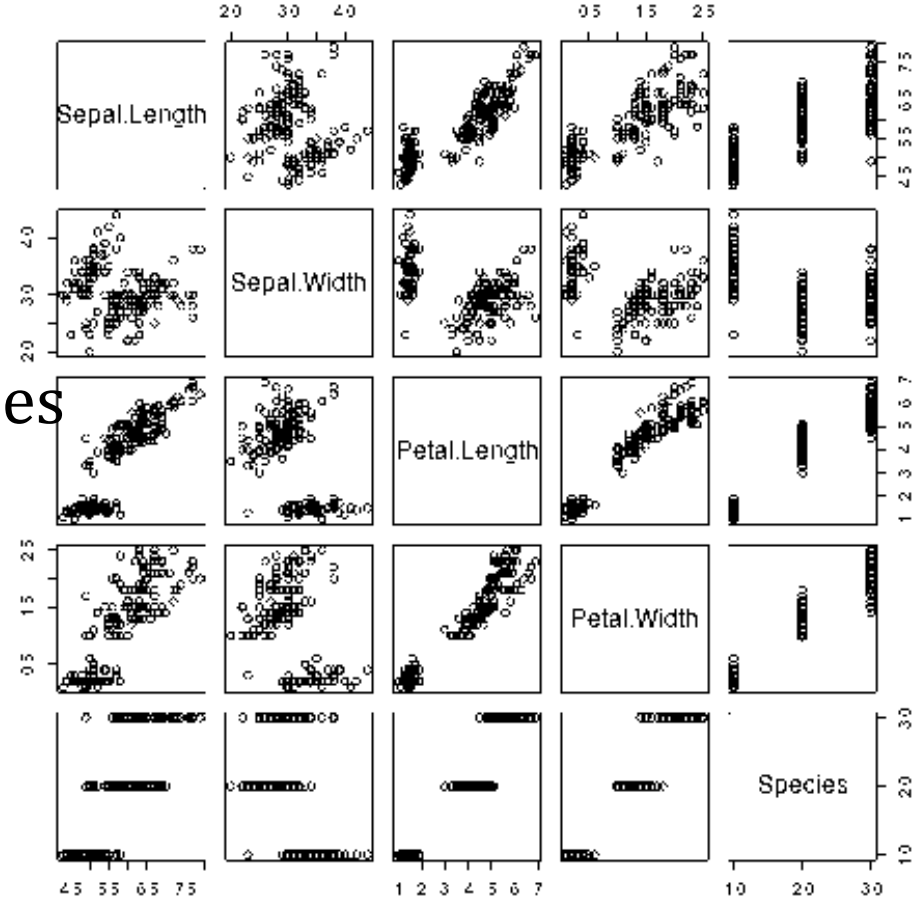
```
> df[2,]
  andrew mary
2  5     6   # a data frame
```

You like scalars, vectors, matrices

- can you avoid data frames ? No
- ¾ of the time, **`df$a`**, **`df$b`** will do
- why must I learn data frames
  - result of **`read.table()`** and friends
  - R has remarkable defaults…

```
> iris    # data set that comes with R – properties of some flowers
    Sepal.Length Sepal.Width Petal.Length Petal.Width    Species
1            5.1         3.5          1.4         0.2     setosa
2            4.9         3.0          1.4         0.2     setosa
…
> pairs (iris)
```

- eats a data frame,
- plots all possible pairs
- no tricks – default plot, default axis scales
- tells me
  - who is correlated with who
  - I should replot without species



# language syntax - for, while, if – no surprises

```
for (i in 1:4) {          # Vorsicht  not for (i=0; i<4; i++)
     i <- i + 10
     print (i)
}
-------------------------------------
i <- 0
while (i < 5){
     print(i)
     i <- i + 1
}
---------
if (i > 3) {
    print('Yes')
} else {
    print('No')
}
```

# functions

```
junk$ Rscript z.r
answer is  18
```

- pass by value
- very often operate on whole vectors

```
$ cat f.r
addup <- function (x) {
      s <- 0
      for (i in x) {
            s = i + s
      }
      return (s)
}

b = c(5, 6, 7)
t <- addup (b)
cat ("answer is ", t, "\n")
```

# Built in functions

- many × $10^2$
- expected maths – trigonometry, logarithms – easy, act on vectors
- type manipulation **`as.vector`**, **`cbind`**, **`rbind`**, .. – foreign and varied
- plotting
- printing (ugly)
- data in / out
- character / text manipulation

- what is the syntax like ? How to read the manual pages ?

# function parameters

- `?log`

```
Usage:
      log(x, base = exp(1))
   ...
```

- log() takes two arguments, $\log(x, b)$ so $\log(x, 10)$ is $\log_{10} x$
- there is a default for the second argument so `log(x)` is really $\ln x$

- a horrible, but important example

`?read.table`

```
read.table(file, header = FALSE, sep = "", quote = "\"'",
      dec = ".", numerals = c("allow.loss", "warn.loss", "no.loss"),
      row.names, col.names, as.is = !stringsAsFactors,
      na.strings = "NA", colClasses = NA, nrows = -1,
      skip = 0, check.names = TRUE, fill = !blank.lines.skip,
      strip.white = FALSE, blank.lines.skip = TRUE,
      comment.char = "#",
      allowEscapes = FALSE, flush = FALSE,
      stringsAsFactors = default.stringsAsFactors(),
      fileEncoding = "", encoding = "unknown", text, skipNul = FALSE)
```

- `read.table('fname')` will often work
- `read.table('fname', skip = 3)` to jump over the first three lines
- …

# Plotting

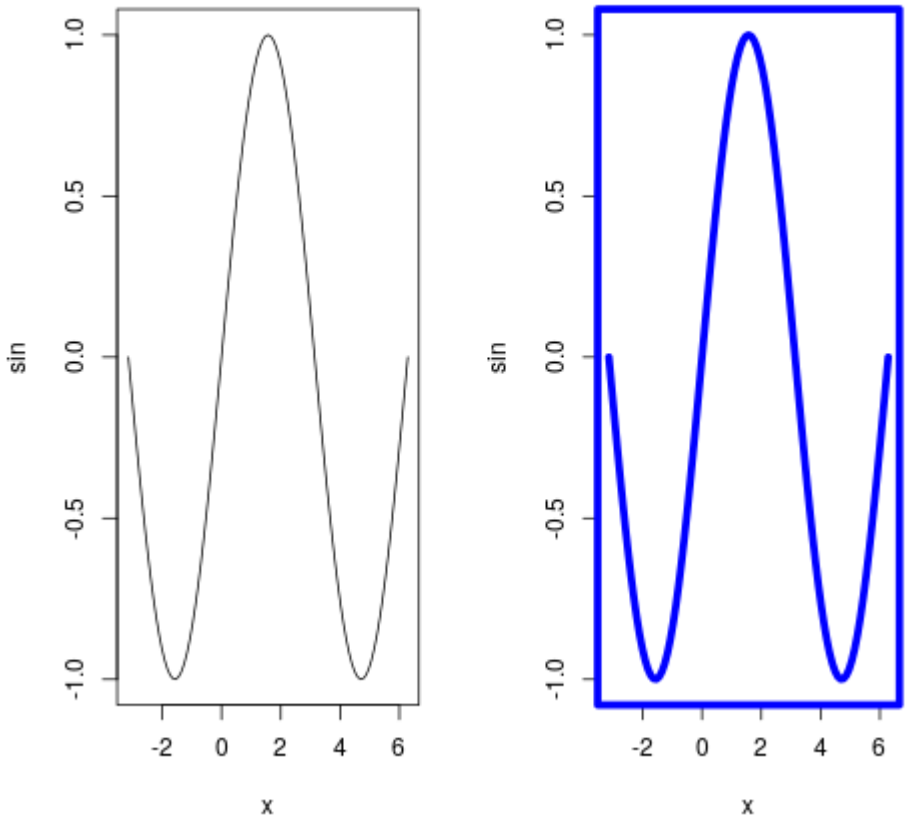
- just the main points
- base R – very clever
  - packages to make it more beautiful `library(ggplot2)`, `library(tidyverse)`
- types ?
  - lines, points, boxes
  - histogramming
  - box +whiskers
  - contours
- what are the surprises ?

# plot complications parameter

Syntax is not pretty – so many parameters

- call **`par()`** and then plot

```
par (mfcol=c(1,2))
plot (sin, -pi, 2*pi)
par (col = "blue", lwd = 5)
plot (sin, -pi, 2*pi)
```



# devices

- do not ever send me a screen dump
- interactive R – no surprises
- usually want output as pdf, png, svg

```
png (file='x.png')
plot (sin, -pi, 2*pi)
dev.off()
```

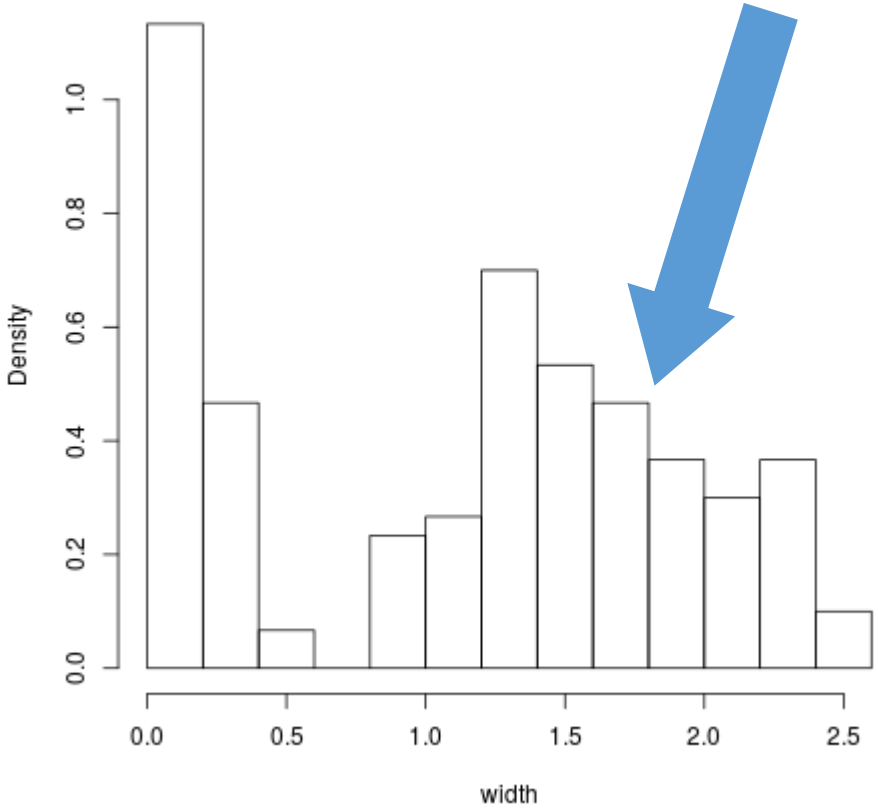
many

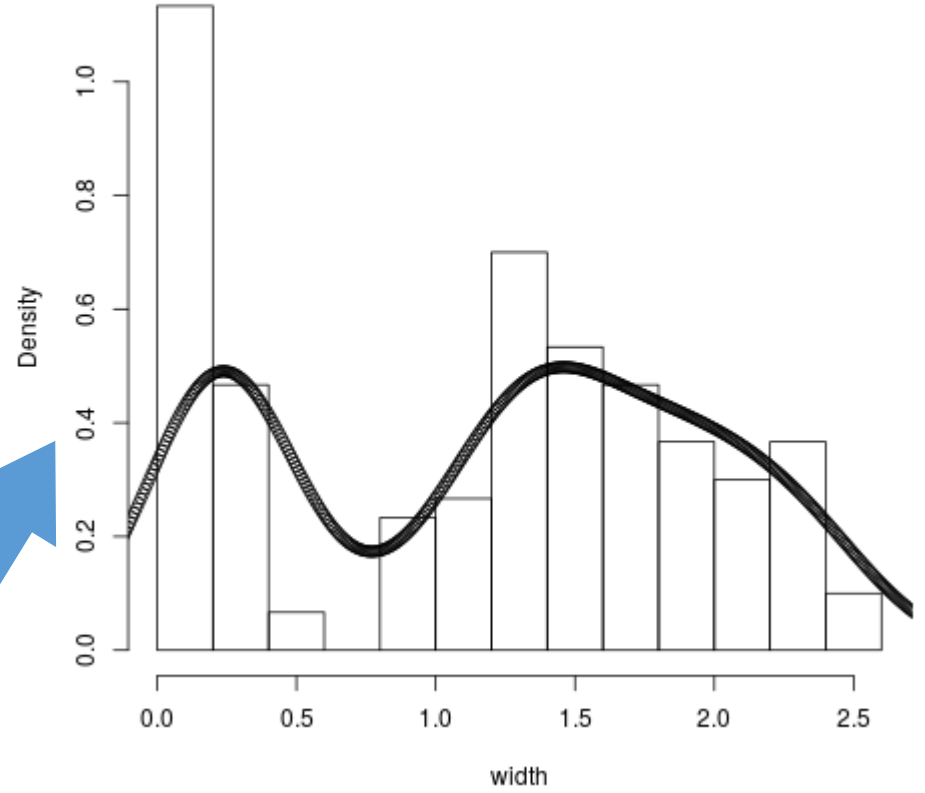
- options
- devices

# Plots are often layered

iris is just a test data set

```
hist (iris$Petal.Width, freq=FALSE, main="", xlab="width")
```




```
hist (iris$Petal.Width, freq=FALSE, main="", xlab="width")
points(density (iris$Petal.Width))
```

# Enough syntax

Next week

- some statistics, fitting, ..