10. Interfacing R

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Interfacing R

With Bioconductor, R can do a huge proportion of the analyses you'll want − but not everything;

- Intensive (or anachronistic) C++, FORTRAN work, e.g. for pedigrees

- 'Speciality' analyses; some need different computing architecture

- Fancy interactive graphics

However, R can be used to 'manage' other software. In this session, we'll illustrate the basic idea with some favorite examples.

Starting other software

NB these commands are for Windows only; see help files for e.g. Unix versions

- `shell()` does the equivalent of a DOS-style command

- `shell("notepad")` starts the Notepad editor

- If the command takes arguments, put them in the same string;
  `shell("notepad myfile.txt")`

The `system()` and `shell.exec()` commands do much the same thing.

Starting other software

Some more options for `shell()`;

- `wait`; R 'hangs' until completion

- `translate`; makes forward and backslashes work properly

- `intern`; return the output as an R object

For other options see the `system()` help page, for example `minimized=TRUE`.

Paths for files can be a little messy; `shell()` starts in your working directory (find it using `getwd()`). For files outside of this, give the full pathway.

`paste()` is useful, if you need to do a lot of this sort of thing.

Examples

Code for a really mundane job;

```
for(i in 1:100){
    infile <- paste("gene",i,"data.txt", sep="")
    outfile <-  paste("gene",i,"phase.out", sep="")
    shell(paste("PHASE",infile,outfile))
}
```

... this will churn away for hours, although with no error-control.

Why did we use `wait=TRUE` here? (the default)

Examples

- WinBUGS implements Bayesian analyses; it's not super-fast but is very flexible

- It needs special (& clever) architecture to achieve this

- WinBUGS' input, output, graphics are all rather clunky

- R is better; so `R2WinBUGS` calls WinBUGS for the difficult bits, and does all the 'translation' itself

- This is done with (repeated) use of `system()`

(Stan has similar functionality, and more state-of-the-art methods for Bayesian calculations.)

Outline

Many programs already exist to do useful analyses. It is more convenient to call them from R than to rewrite them in R.

Sometimes this involves calling the C code directly, sometimes just involves using R to write input files for another program

Examples:

- Graphviz: drawing networks

- PMF: input files for ancient Fortran software

- Google Earth: displaying outliers in context.

Drawing networks

GraphViz (http://www.graphviz.org) is a free program for drawing networks, written by AT&T researchers.

Its input format looks like

```
"15" [shape= box,regular=1 ,height= 0.5 ,width= 0.75 ,style=filled,color= grey ] ;
"16" [shape= circle ,height= 0.5 ,width= 0.75 ,style=filled,color= grey ] ;
"2x3" [shape=diamond,style=filled,label="",height=.1,width=.1] ;
"2"  ->  "2x3"  [dir=none,weight=1]  ;
"3"  ->  "2x3"  [dir=none,weight=1]  ;
"2x3"  ->  "1" [dir=none,weight=2]  ;
"2x3"  ->  "4" [dir=none,weight=2]  ;
"2x3"  ->  "5" [dir=none,weight=2]  ;
"2x3"  ->  "6" [dir=none,weight=2]  ;
```

The sem package uses GraphViz to display path diagrams for structural equation models and the gap package uses it to draw pedigrees.

Drawing networks

In `gap` the `pedtodot()` function writes a GraphViz input file from a pedigree in GAS or LINKAGE format.

```
    pid id fid mid sex aff GABRB1 D4S1645
1   10081  1   2   3   2   2    7/7    7/10
2   10081  2   0   0   1   1    -/-     -/-
3   10081  3   0   0   2   2    7/9    3/10
4   10081  4   2   3   2   2    7/9     3/7
5   10081  5   2   3   2   1    7/7    7/10
6   10081  6   2   3   1   1    7/7    7/10
7   10081  7   2   3   2   1    7/7    7/10
8   10081  8   0   0   1   1    -/-     -/-
9   10081  9   8   4   1   1    7/9    3/10
10  10081 10   0   0   2   1    -/-     -/-
11  10081 11   2  10   2   1    7/7     7/7
12  10081 12   2  10   2   2    6/7     7/7
13  10081 13   0   0   1   1    -/-     -/-
14  10081 14  13  11   1   1    7/8     7/8
15  10081 15   0   0   1   1    -/-     -/-
16  10081 16  15  12   2   1    6/6     7/7
```

Drawing networks

First the code prints nodes for each individual, with sex and affectedness information

```
for (s in 1:n) cat(paste("\"", id.j[s], "\" [shape=",
    sep = ""), shape.j[s], ",height=", height, ",width=",
    width, ",style=filled,color=", shade.j[s], "] ;\n")
```

giving output like

```
"16" [shape= circle ,height= 0.5 ,width= 0.75 ,style=filled,color= grey ] ;
```

It then works out all the matings and creates small nodes for each mating and lines connecting the parents to these nodes

```
mating <- paste("\"", s1, "x", s2, "\"", sep = "")
cat(mating, "[shape=diamond,style=filled,label=\"\",height=.1,width=.1] ;\n")
cat(paste("\"", s1, "\"", sep = ""), " -> ", mating,
    paste(" [dir=", dir, ",weight=1]", sep = ""),
     " ;\n")
cat(paste("\"", s2, "\"", sep = ""), " -> ", mating,
    paste(" [dir=", dir, ",weight=1]", sep = ""),
    " ;\n")
```
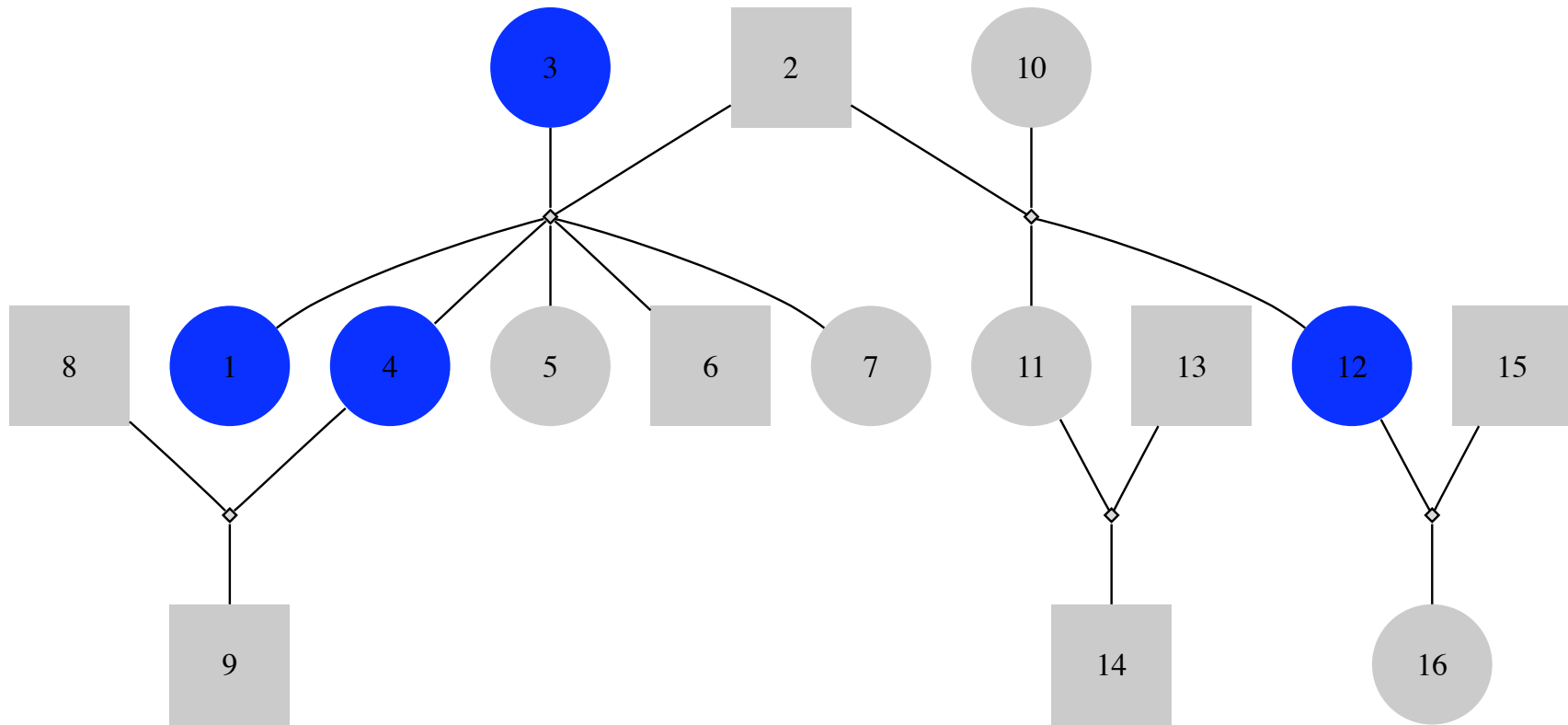
Drawing networks

giving output like

```
"2x3" [shape=diamond,style=filled,label="",height=.1,width=.1] ;
"2"  ->  "2x3"  [dir=none,weight=1]  ;
"3"  ->  "2x3"  [dir=none,weight=1]  ;
```

and then connects children to parents.

Drawing networks

pedigree 10081

[Bioconductor also has GraphViz more integrated with R in the
`RGraphViz` package]

Chromosome simulation

MaCS, the Markov Coalescent Simulation (Chen et al, 2008) simulates realistic genotypes using an approximation to the coalescent.

It's a command-line program written in C++, with output:

```
/Users/tlumley/macs/macs 2000 15000 -t .001 -r .001 .001
1390319964

//
segsites: 134
positions: 0.000421536259 0.0100671644 0.0111485623 0.0230004096 0.0332452159...
10000000000000000000000000010010001000100000000000000000001010000...
00000000000000000000000000000000000000000000000000000000000000000...
00000000000000000000000000000000000000000000000000000000000000000...
```

We want the same sort of simulation functions as in earlier sessions, so we need an R function that calls MaCS, and returns a data matrix.

Chromosome simulation

Tasks

- Call MaCS

- Read in the lines of haploid genotypes as character strings

- Split into numbers

- Recode so 1 is the minor allele

- Combine pairs of haploids into a diploid

Chromosome simulation

```r
makemacsdata<-function(N,length=15000,filter=0.05){
  f<-tempfile()
  system(paste("~/macs/macs",2*N,length,
      " -t .001 -r .001 2>/dev/null | ~/macs/msformatter >", f))
  input<-readLines(f)[-(1:6)]
  unlink(f)
  haplo<-do.call(rbind,lapply(strsplit(input,""),as.integer))
  diplo<-haplo[1:N,]+haplo[(N+1):(2*N),]
  af<-colMeans(diplo)/2
  diplo[,af>0.5]<- 2-diplo[,af>0.5,drop=FALSE]
  maf<-colMeans(diplo)/2
  diplo[,af<=filter,drop=FALSE]
}
```

Chromosome simulation

From the user's viewpoint it looks as though everything was done in R;

```
> d <- makemacsdata(1000)
> str(d)
 num [1:1000, 1:80] 0 0 0 0 0 0 0 0 0 0 ...
> summary(colMeans(d)/2) #maf
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
0.00050 0.00100 0.00450 0.01142 0.01512 0.05000
```

Chromosome simulation

Now simulate a new version of the SKAT rare-variant test;

```
one.sim<-function(thresholds=c(Inf,1/2,1/3,1/4),
        sqrtweights=wuweights,
        N=4000, n=200, length=15000, filter=0.02)
{
  G <- makemacsdata(N,length,filter=filter)
  y <- sample(rep(0:1,c(N-n,n)))
  sapply(thresholds,
      function(c) winskat(G,y,threshold=c,sqrtweights))
}
```

SVG+tooltips

SVG (Scalable Vector Graphics) is a non-bitmap graphics format for the web.

The `RSvgDevice` and `RSVGTipsDevice` packages allow R output to SVG format.

We can use this to create graphs with links and tooltips. For example, a funnelplot showing associations between a large number of SNPs and VTE.

Point at a dot to see the SNP it represents, and click to go to information about the gene.

SVG+tooltips

```
for(i in 1:length(or)) {
    setSVGShapeToolTip(title=gene[i],
        desc1=snp[i],
        desc2=if(abs(lor[i]/se[i])>qnorm(0.5/n,lower.tail=FALSE))
                            qvals[i] else NULL
    )

    setSVGShapeURL(paste("http://pga.gs.washington.edu/data",
                                tolower(gene[i]),
                                sep="/")
        )
    points(prec[i],lor[i], cex=1, pch=19, col='grey')
}
```

Google Earth

Google Earth is controlled by KML files specifying locations. KML is another plain text format.

Using `cat()`, we can write a short KML file;

```
<?xml version="1.0" encoding="UTF-8"?>
        <kml xmlns="http://earth.google.com/kml/2.1">
        <Placemark>
        <name> 1 </name>
  <Point> <coordinates>-118.0256,34.11619,400</coordinates>
  </Point>
 </Placemark>
</kml>
```
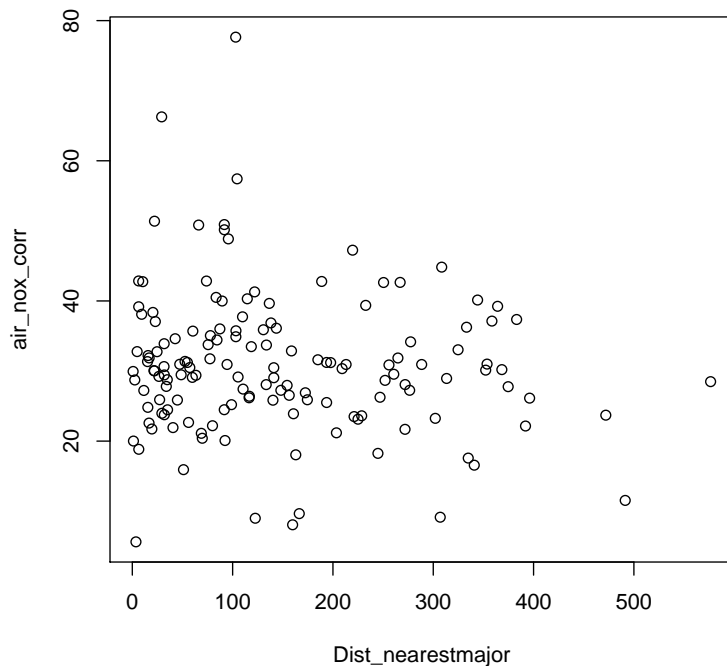
and then send it to Google Earth with the `shell.exec(filename)` function, which opens a file using whatever is the appropriate program.

Google Earth

Finally, the `identify()` function lets the user select a point on a scatterplot;

In this example the points are locations where air pollution was measured, and we can call Google Earth to look at the location.