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

`R` can be used to 'manage' other software. Today we'll illustrate
some favorite examples

Starting other software

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

- `system` is the equivalent of a DOS-style command

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

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

The `shell` command does much the same thing.

Starting other software

Some more options for `system`;

- `wait`; R 'hangs' until completion

- `minimized`; new program only appears in TaskBar

- `show.output.on.console`

Paths for files can be a little messy; `system` starts in your working directory (`getwd`). Outside of this, give the full pathway.

`paste` is useful, if you need to do a lot of this sort of thing. `source` may also help

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="")
    system(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 analyse; 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()`

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")
```
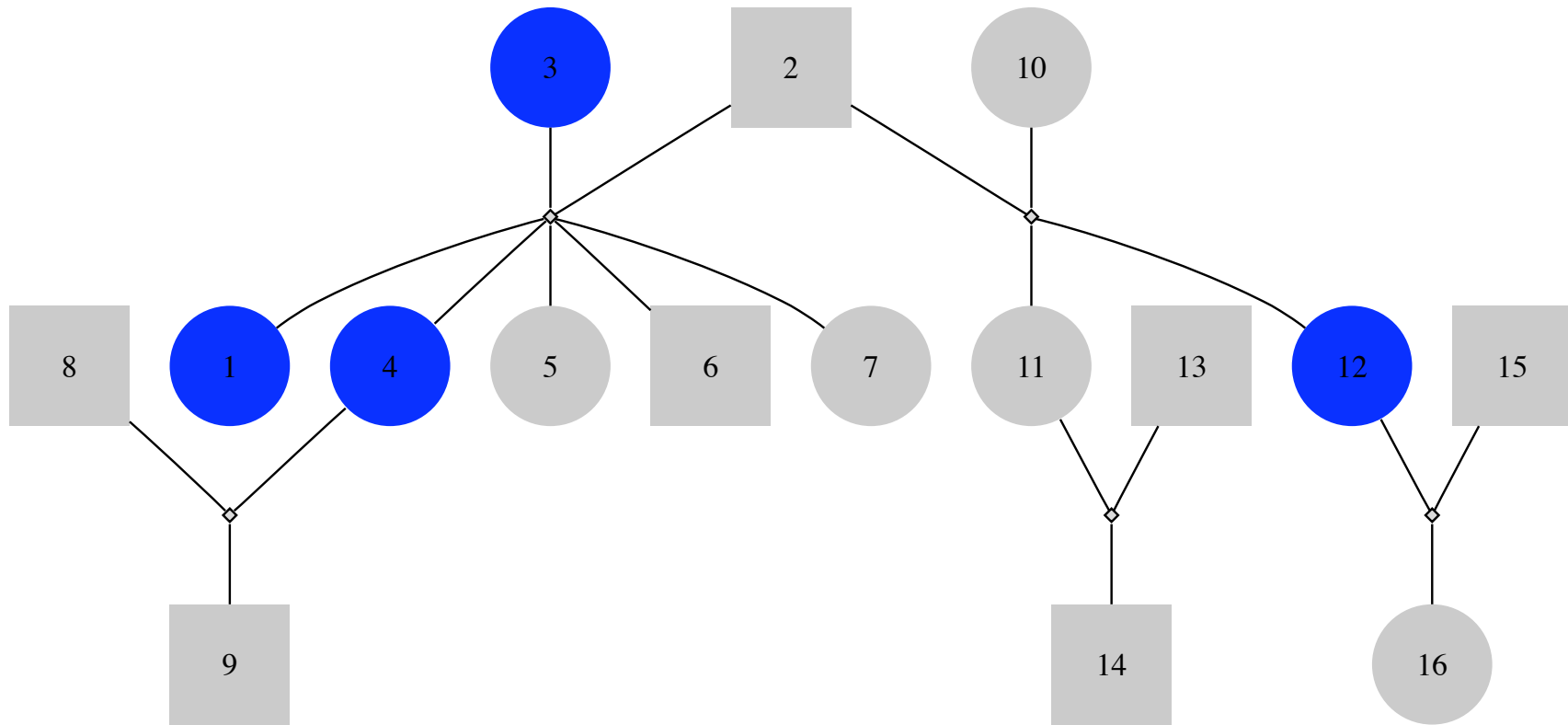
Drawing networks

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]

PMF: factor analysis

PMF is a program for constrained factor analysis in analytic chemistry. It is controlled by an ugly text input file:

```
pmfini<-c(" ##PMF2 .ini file for: Simulations from R",
" ## Monitor code M: if M>1, PMF2 writes output every Mth step",
" ## For finding errors, use M<1 to output debug information",
" ##       M        PMF2 version number",
"        1          4.2",
" ## Dimensions: Rows, Columns, Factors. Number of \"Repeats\"",
"              @nt@        @ns@          @sources@         1",
" ##   \"FPEAK\"  (>0.0 for large values and zeroes on F side)",
"     @FPEAK@",
" ## Mode(T:robust, F:non-robust)  Outlier-distance        (T=True F=False)",
"          @isrobust@                          @outlier@",
" ## Codes C1 C2 C3 for X_std-dev, Errormodel EM=[-10 ... -14]",
"        0.0100    0.0000    0.0100      -12",
" ## G Background fit:  Components   Pullup_strength",
"                            0        0.0000",
" ## Pseudorandom numbers:   Seed     Initially skipped",
"                          @seed@          0",
" ## Iteration control table for 3 levels of limit repulsion \"lims\"",
```

The `@value@` are places where we want to substitute in a value.

PMF: factor analysis

R code for the substitutions looks like

```
temp<-gsub("@FPEAK@",formatC(fpeak,digits=4,format="f"),pmfini)
temp<-gsub("@isrobust@",isrobust,temp)
seed<-as.character(as.integer(seed))
temp<-gsub("@seed@", seed, temp)
```

PMF: factor analysis

We can write data files needed by PMF, and then write the control file, then call PMF with the `system()` function. After PMF finishes we read in the results.

```
write.table(cX,file=xfile, quote=FALSE, col.names=FALSE, row.names=FALSE)
write.table(cU,file=efile, quote=FALSE, col.names=FALSE, row.names=FALSE)
if (!debug)
    on.exit(unlink(c(xfile,efile,inifile)))
writeLines(temp,inifile)

sysval<-system(paste(pmf,inifile), intern=TRUE,invisible=!debug)

ffactor<-read.table(outfiles$f,row.names=sourcenames,col.names=species)
gfactor<-read.table(outfiles$g,row.names=times,col.names=sourcenames)
```

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

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.

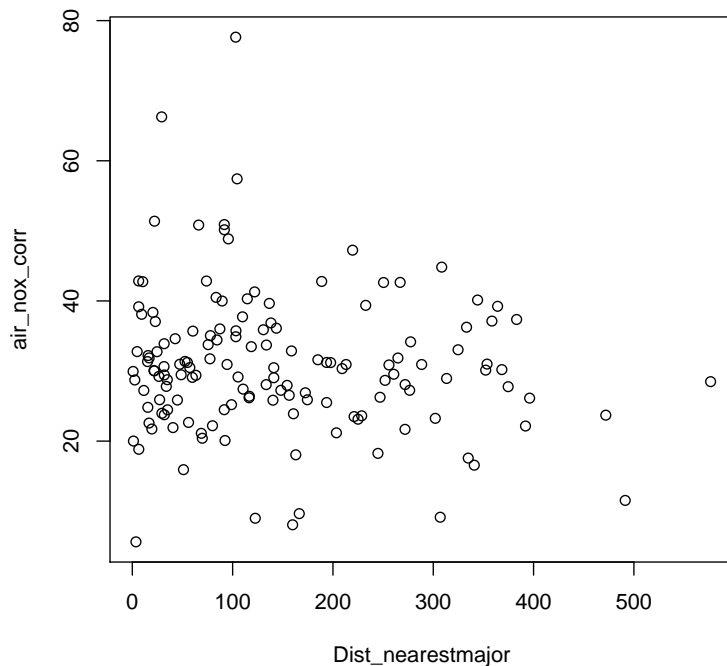We can write a KML file

```
<?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

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.