Scientific Programming Assignment 2

MPhil in Computational Biology

October 26, 2021

If there are errors found, I will update the assignment on the web at `http://github.com/sje30/sp2021`

Due date: 2021-11-10 23:45

Please submit your report to Moodle as a Rnw: NO OTHER FORMATS ARE ACCEPTED.

Name your file `spa2_XXX.Rnw`, where XXX is your unique code. The files will be marked anonymously so please refrain from writing your name (or CRSid) in the document.

You must ensure that the file can be compiled into a PDF by someone else using:

```
require(knitr); knit2pdf('spa2_XXX.Rnw')
```

Your .Rnw file should dynamically compute and report answers, rather than you writing the code and then typing your answers manually into the latex part of the document. In particular, it should run on subliminal, using only the system packages installed. If in doubt about whether you can use a given package, ask me in advance. (You may use .Rmd, rather than .Rnw as long as you indicate clearly how to convert it to a pdf.)

Your report must be a maximum of ten pages, excluding the appendix. This course work will consist of 30% towards your overall mark for this module.

1 Permutations [5 marks]

Write a *recursive* function that generates all $N!$ permutations of a vector of length N. The output should be a matrix, one permutation per row. For example, with three elements:

```
permutations(1:3)
```

```
##      [,1] [,2] [,3]
## [1,]    1    2    3
## [2,]    1    3    2
## [3,]    2    1    3
## [4,]    3    1    2
## [5,]    2    3    1
## [6,]    3    2    1
```

Demonstrate it working on the vector `1:4`. Verify that it generates the correct outputs when given the input vector `1:6`.

```
par(mfrow=c(1,2),mar=c(2,2,1.5,1))
skyplot( 1:20, 1:25, main='A')
skyplot( c(2,0,0,0,2,  0,0,0,2,0,  0,0,3,4,0,  0,1,0,2,0),
         c(0,0,0,0,0,  0,0,0,0,0,  0,0,0,0,5,  5,0,0,0,4, 0,0,0,0,0),
         main='B')
```

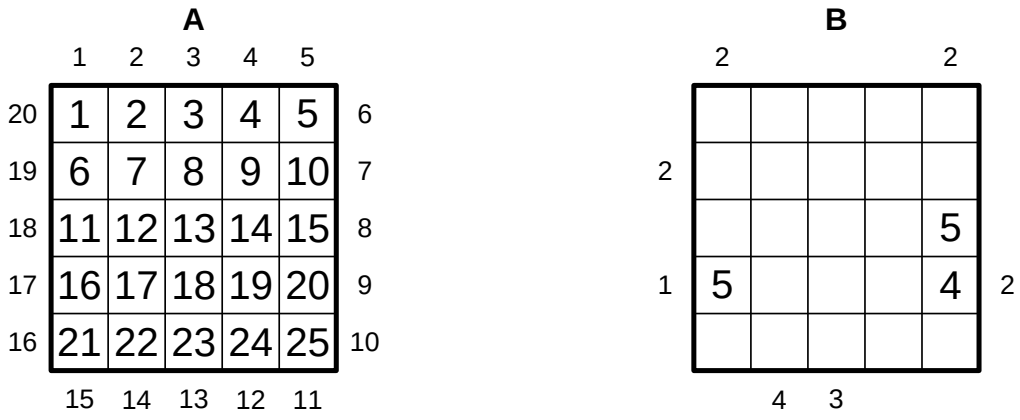

Figure 1: Layout of the skyscraper problem. Panel A shows the indexing used. Panel B shows a typical 5x5 problem.

2 Skyscraper [10 marks]

`https://www.brainbashers.com/skyscrapers.asp`. Your job is to solve the skyscraper puzzle.

1. Write the function "skyplot" that draws the skyscraper problem for N=4–9. Use your function to draw the two grids shown in Figure 1. It should have the following structure:

```
skyplot <- function(edges, soln, ...) {
  ## EDGES is a vector of length 4N containing the numbers clockwise
  ## around the grid, starting in the top left corner.  SOLN is a
  ## vector of length N^2, storing on a row-by-row basis, starting in
  ## top-left corner.  Any elements containing 0 are meant to indiciate blank.
  ## N could be between 4 and 9.
  ...
}
```

2. Write a solver for the case $N = 4$. Show all the solutions to the problems in Figure 2. Show your answers using the skyplot() function to draw sky plots. [5 marks]

Hints: to solve this problem, the search space is small enough that you can exhaustively search all possible solutions using your answer to question 1. For drawing primitives, look at the functions: *segments(), text()*.

```
par(mfrow=c(1,2),mar=c(2,2,1.5,1))
e1 = scan(comment.char="#", quiet=T,
              'https://raw.githubusercontent.com/sje30/sp2021/main/assigns/skyscraper.dat')
skyplot(e1, rep(0,16), main='A')
e2 = c(3,0,1,0, 0,0,1,0, 0,0,0,0, 0,0,0,2)
skyplot(e2, rep(0,16), main='B')
```

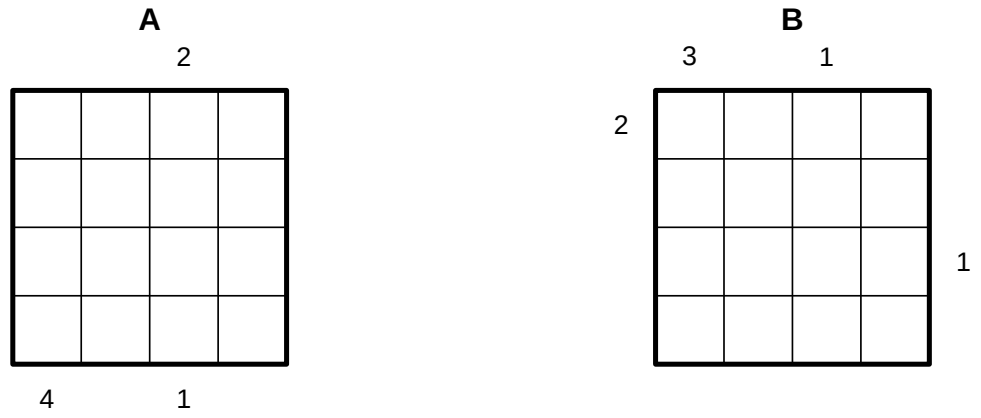

Figure 2: Solve these problems. Ensure that you read in e1 as above, as I **may** change this file when compiling your pdf. (If it changes, you can assume it will be a valid 4x4 problem.)

3 Simulated annealing [15 marks]

(a) Download and use the R code from
`http://toddwschneider.com/posts/traveling-salesman-with-simulated-annealing-r-and-shiny/`
to solve the travelling salesman problem for the points stored in the file
`https://raw.githubusercontent.com/sje30/sp2021/main/assigns/cambridgecolleges.txt`.

What is your optimum tour length and how does it compare to that from Concorde `https://neos-server.org/neos/solvers/co:concorde/TSP.html`? [5 marks]

(b) Use simulated annealing to solve the following Magic 19 puzzle (from NRICH). "Label the dots [in the hexagon of Figure 3] with the numbers 1 to 19 so that each set of three dots that lie along a straight-line segment add up to 22."

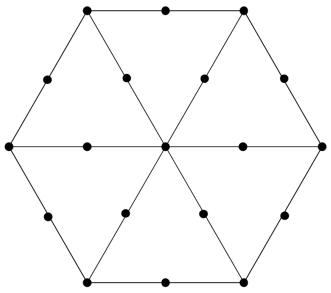

Figure 3: Magic 19 puzzle

Describe your energy function, new state selection, annealing schedule and any other relevant details. How many solutions can you find? [10 marks]