

CT561: Systems Modelling & Simulation

Lecture 9: Exploring Models in R

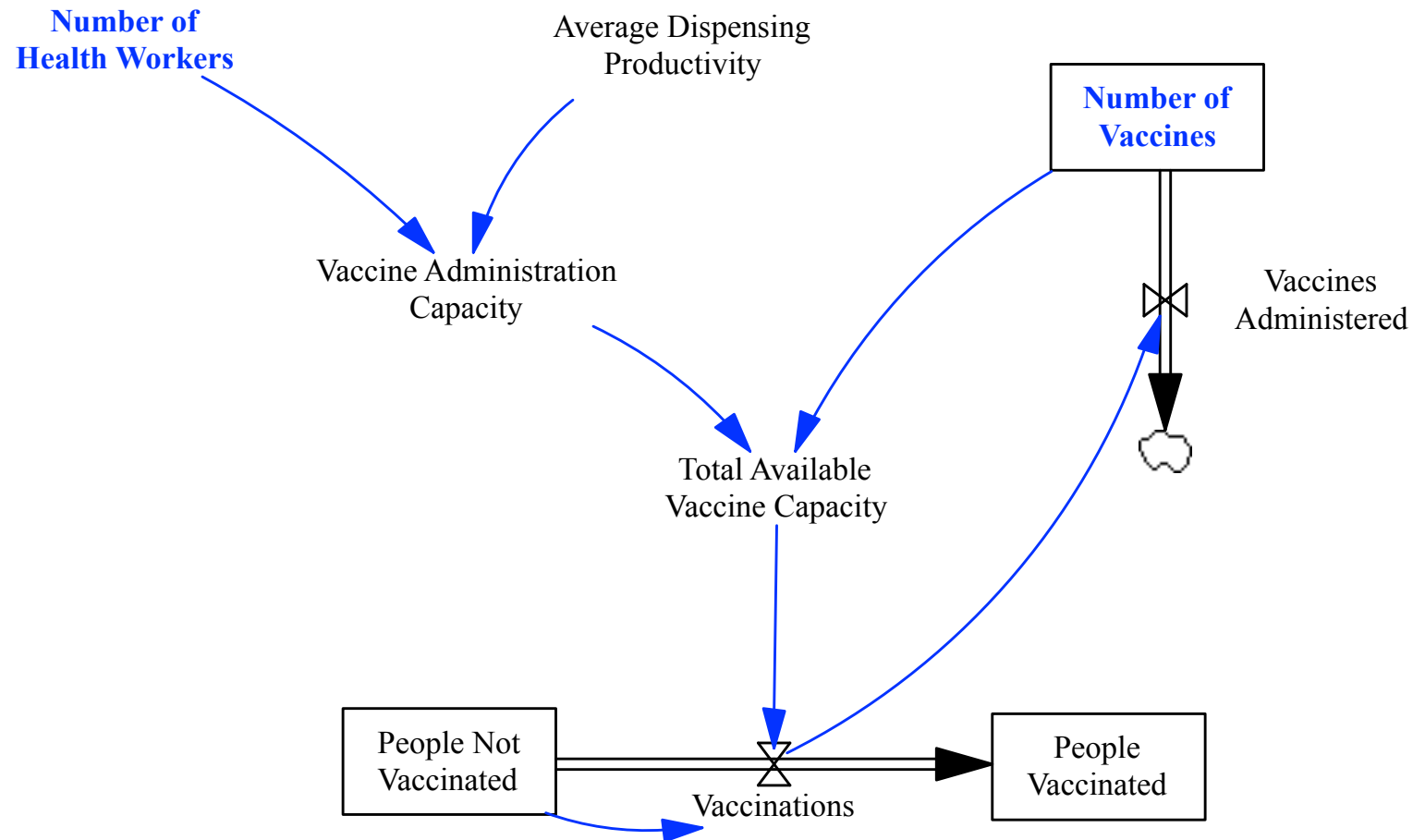
Dr. Jim Duggan,
School of Engineering & Informatics
National University of Ireland Galway.

<https://github.com/JimDuggan/SDMR>

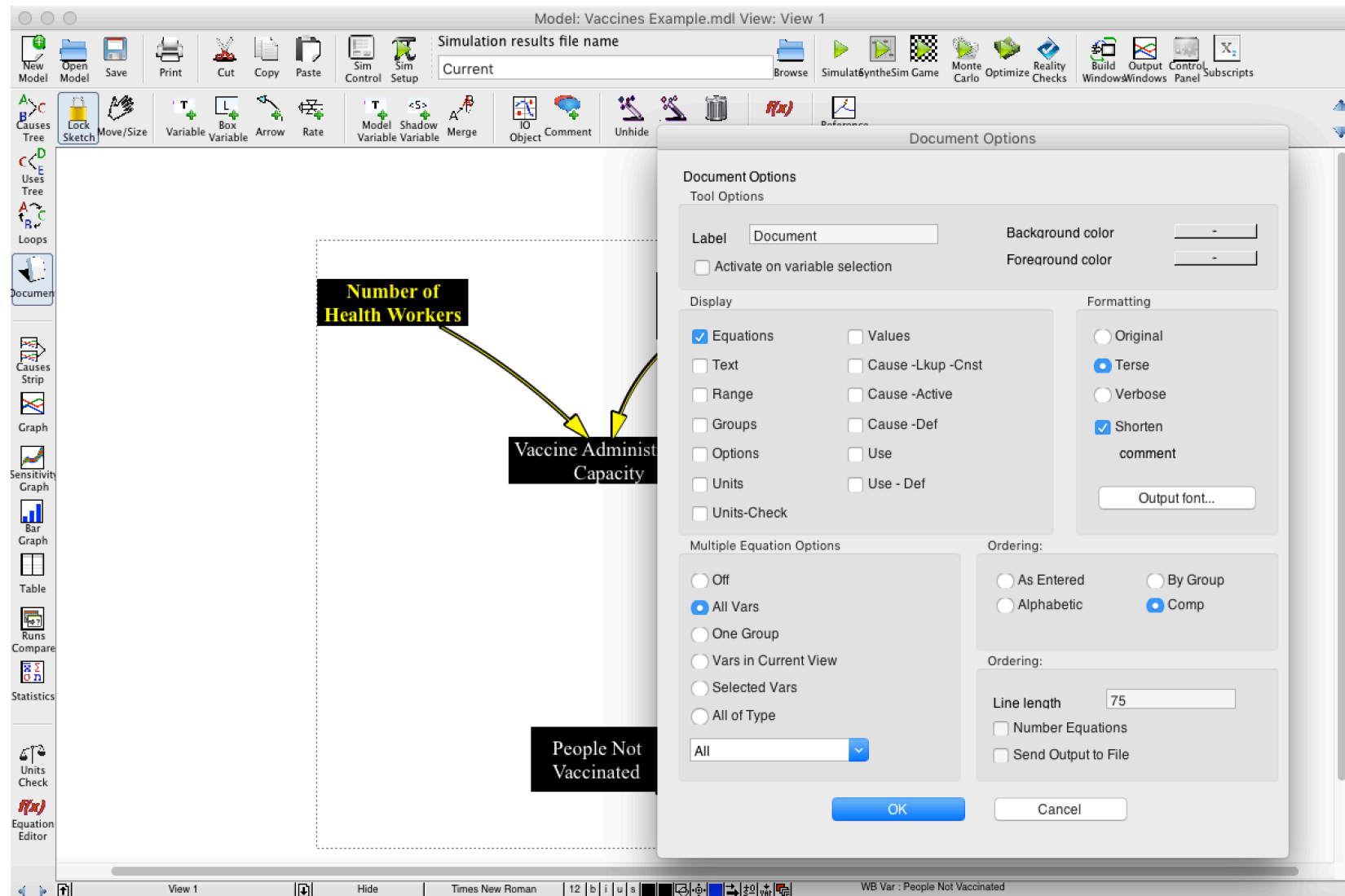
https://twitter.com/_jimduggan



Translation Utility (Vensim – deSolve)



Vensim Document Options



Select equations...

Model: Vaccines Example.mdl View: View 1

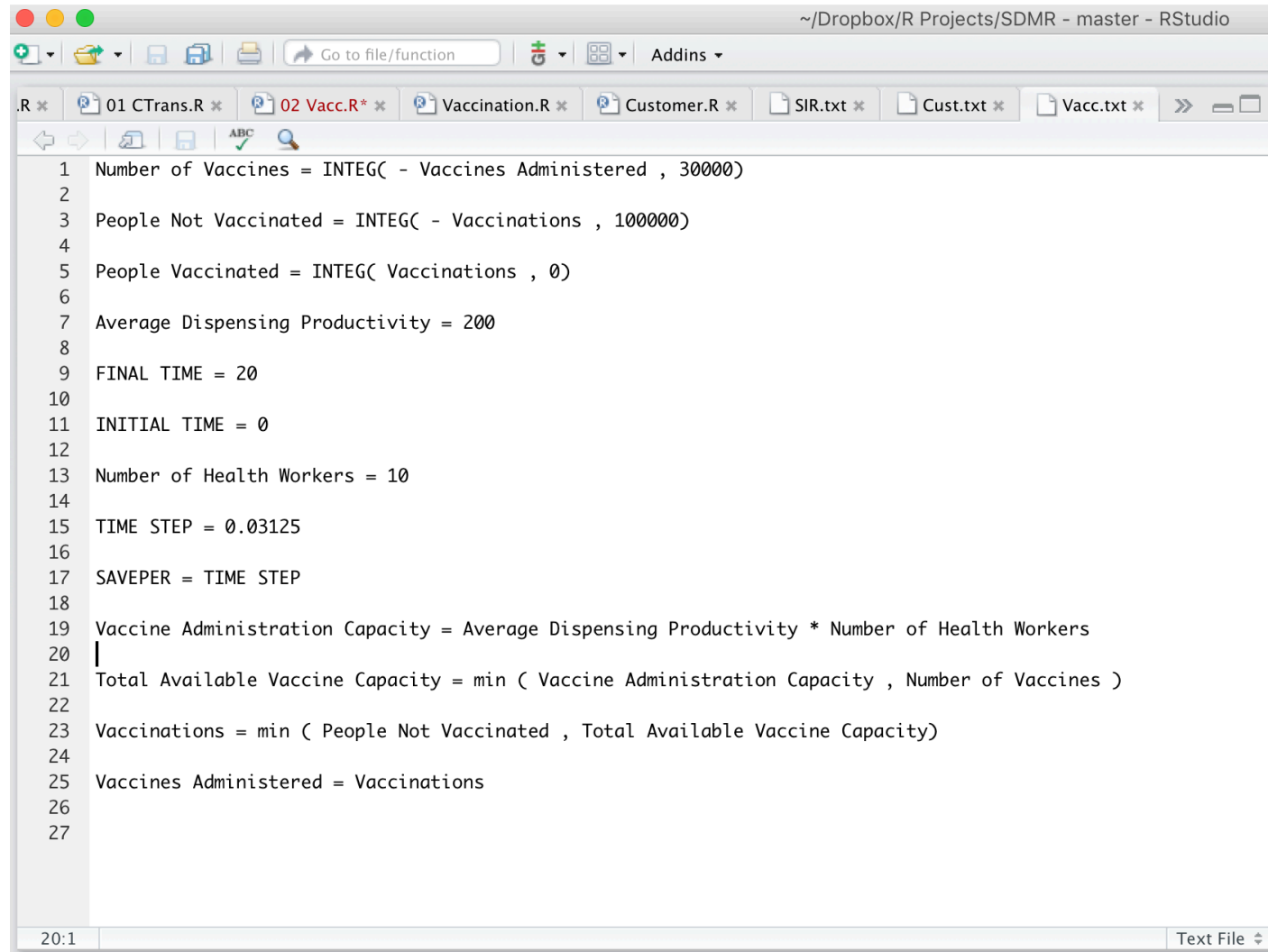
Simulation results file name: Current

Equations:

```
Number of Vaccines = INTEG( - Vaccines Administered , 30000)
People Not Vaccinated = INTEG( - Vaccinations , 100000)
People Vaccinated = INTEG( Vaccinations , 0)
Average Dispensing Productivity = 200
FINAL TIME = 20
INITIAL TIME = 0
Number of Health Workers = 10
TIME STEP = 0.03125
SAVEPER = TIME STEP
Vaccine Administration Capacity = Average Dispensing Productivity * Number of Health Workers
Total Available Vaccine Capacity = min ( Vaccine Administration Capacity ,
    Number of Vaccines )
Vaccinations = min ( People Not Vaccinated , Total Available Vaccine Capacity )
Vaccines Administered = Vaccinations
```

Diagram: People Not Vaccinated → Vaccinations → People Vaccinated

Copy into Rstudio and save (Vacc.txt)



The screenshot shows the RStudio interface with a script editor open. The title bar indicates the path is ~/Dropbox/R Projects/SDMR - master - RStudio. The script editor contains the following R code:

```
1 Number of Vaccines = INTEG( - Vaccines Administered , 30000)
2
3 People Not Vaccinated = INTEG( - Vaccinations , 100000)
4
5 People Vaccinated = INTEG( Vaccinations , 0)
6
7 Average Dispensing Productivity = 200
8
9 FINAL TIME = 20
10
11 INITIAL TIME = 0
12
13 Number of Health Workers = 10
14
15 TIME STEP = 0.03125
16
17 SAVEPER = TIME STEP
18
19 Vaccine Administration Capacity = Average Dispensing Productivity * Number of Health Workers
20 |
21 Total Available Vaccine Capacity = min ( Vaccine Administration Capacity , Number of Vaccines )
22
23 Vaccinations = min ( People Not Vaccinated , Total Available Vaccine Capacity)
24
25 Vaccines Administered = Vaccinations
26
27
```

The status bar at the bottom left shows '20:1' and the bottom right shows 'Text File'.

Create “compiler” file...

```
source("reader/conv_to_deSolve.R")  
  
output<-sim$translate_vensim("./reader/Vacc.txt")  
  
sim$save_model(output, "./reader/Vaccination.R")
```

```

library(deSolve)
library(ggplot2)
library(reshape2)
#Displaying the simulation run parameters
START_TIME <- 0.000000
FINISH_TIME <- 20.000000
TIME_STEP <- 0.031250
#Setting aux param to NULL
auxs<-NULL

#Generating the simulation time vector
simtime<-seq(0.000000,20.000000,by=0.031250)
# Writing global variables (stocks and dependent auxs)
stocks <-c( NumberofVaccines = 30000 , PeopleNotVaccinated = 100000 , PeopleVaccinated = 0 )
# This is the model function called from ode
model <- function(time, stocks, auxs){
  with(as.list(c(stocks, auxs)),{
    AverageDispensingProductivity <- 200
    NumberofHealthWorkers <- 10
    VaccineAdministrationCapacity <- AverageDispensingProductivity*NumberofHealthWorkers
    TotalAvailableVaccineCapacity <- min(VaccineAdministrationCapacity,NumberofVaccines)
    Vaccinations <- min(PeopleNotVaccinated,TotalAvailableVaccineCapacity)
    VaccinesAdministered <- Vaccinations
    d_DT_NumberofVaccines <- -VaccinesAdministered
    d_DT_PeopleNotVaccinated <- -Vaccinations
    d_DT_PeopleVaccinated <- Vaccinations
    return (list(c(d_DT_NumberofVaccines,d_DT_PeopleNotVaccinated,d_DT_PeopleVaccinated)))
  })
}
# Function call to run simulation
o<-data.frame(ode(y=stocks,times=simtime,func=model,parms=auxs,method='euler'))

```

Resource on github: /reader

JimDuggan / SDMR

Unwatch 1 Star 3 Fork 4

Code Issues 0 Pull requests 0 Projects 0 Wiki Pulse Graphs Settings

Branch: master SDMR / reader / Create new file Upload files Find file History

JimDuggan Adding Vaccination example from lectures Latest commit 6168d2d 6 minutes ago

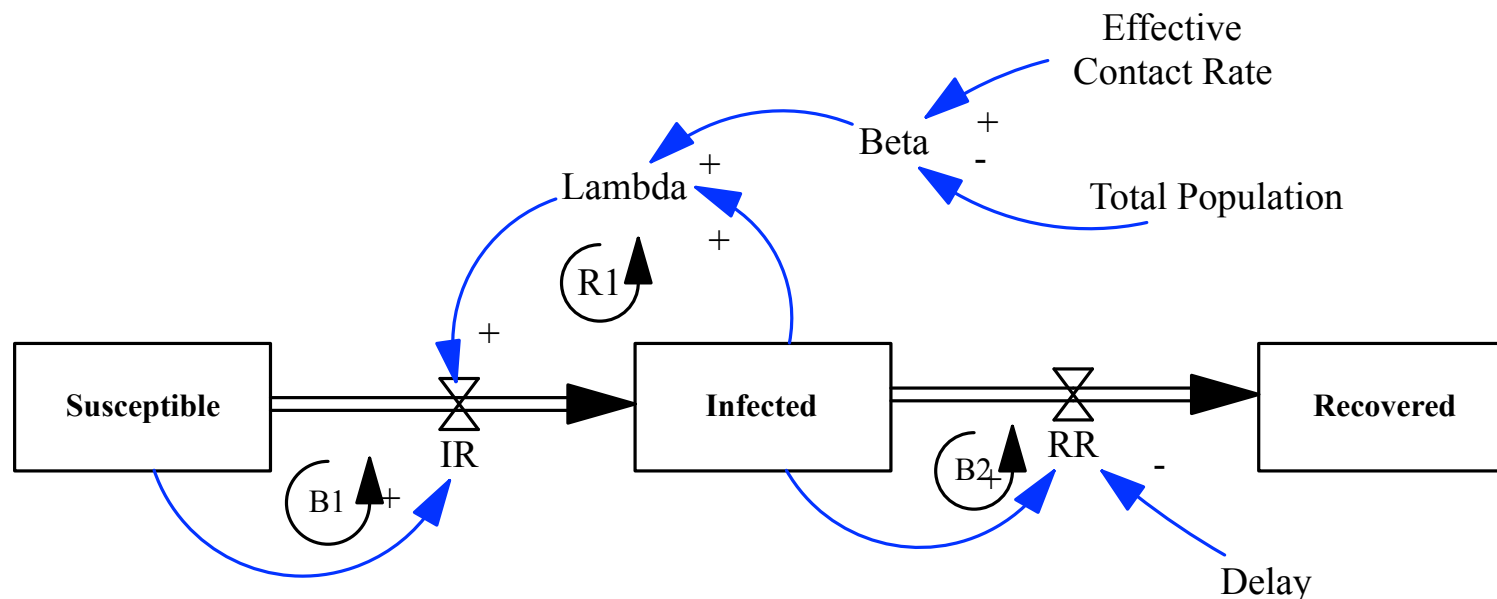
..

01 CTrans.R	Updating reader to filter out blank lines...	3 hours ago
02 Vacc.R	Adding Vaccination example from lectures	6 minutes ago
Current.vdf	Adding lecturing archive from 2015	3 months ago
Cust.txt	Updating reader to filter out blank lines...	3 hours ago
Customer.R	Updating reader to filter out blank lines...	3 hours ago
SIR Vensim.2mdl	Update...	3 months ago
SIR Vensim.mdl	Update README doc...	3 months ago
SIR.R	Updating reader to filter out blank lines...	3 hours ago
SIR.txt	Update README doc...	3 months ago
TestScript.R	Updating test script...	3 months ago
Vacc.txt	Adding Vaccination example from lectures	6 minutes ago



Exploratory Model Analysis – SIR Model

Diffusion - a fundamental process in physical, biological, social and economic settings (Rahmandad and Sterman 2008).



Sensitivity Analysis (library FME)

- Vary key parameters
 - Effective Contacts
 - Recovery Delay
- Perform many simulation runs
- Analyse output

Package ‘FME’

February 19, 2015

Version 1.3.2

Title A Flexible Modelling Environment for Inverse Modelling, Sensitivity, Identifiability, Monte Carlo Analysis.

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Maintainer Karline Soetaert <karline.soetaert@nioz.nl>

Depends R (>= 2.6), deSolve, rootSolve, coda

Imports minpack.lm, MASS

Suggests diagram

Description Provides functions to help in fitting models to data, to perform Monte Carlo, sensitivity and identifiability analysis. It is intended to work with models be written as a set of differential equations that are solved either by an integration routine from package deSolve, or a steady-state solver from package rootSolve. However, the methods can also be used with other types of functions.



Overall Idea

R Source code

Run Simulation Function (params)

Model function

Net flow equations go here

**Call Model Function
Return Results**

**Setup Params (FME library)
Call Simulation Function
Display Results**



Generating Parameters

```
CE.MIN<-0;          CE.MAX<-7.0
DEL.MIN<-1.0;       DEL.MAX<-10.0
INIT.INF.MIN<-1.0;  INIT.INF.MAX<-25.0;

parRange<-data.frame(
  min=c(CE.MIN, DEL.MIN, INIT.INF.MIN),
  max=c(CE.MAX, DEL.MAX, INIT.INF.MAX)
)

rownames(parRange)<-c("aEffective.Contact.Rate", "aDelay", "initInfected")

NRUNS<-10
p<-data.frame(RunNo=1:NRUNS, Latinhyper(parRange, NRUNS))
```

parRange data frame & LatinHyper()

```
> parRange
```

	min	max
aEffective.Contact.Rate	0	7
aDelay	1	10
initInfected	1	25

```
>
```

```
> p
```

	RunNo	aEffective.Contact.Rate	aDelay	initInfected
1	1	5.7435887	4.635804	13.738034
2	2	3.0020634	8.499875	22.389610
3	3	0.8393408	2.684578	17.206845
4	4	2.5906431	7.061717	12.551525
5	5	0.0264442	9.213793	23.679345
6	6	4.2287664	8.193284	8.757535
7	7	6.8971697	4.544439	5.548590
8	8	5.5252311	5.864802	2.606257
9	9	1.8602947	3.583974	7.451173
10	10	3.8608469	1.207800	17.882494

Overall idea... N simulation runs

> p

	RunNo	aEffective.Contact.Rate	aDelay	initInfected
1	1	5.7435887	4.635804	13.738034
2	2	3.0020634	8.499875	22.389610
3	3	0.8393408	2.684578	17.206845
4	4	2.5906431	7.061717	12.551525
5	5	0.0264442	9.213793	23.679345

Run Simulation Function (params)

Model function

Net flow equations go here

Call Model Function
Return Results

The Code (1/3)

```
runsim <- function(rvec){  
  # this is the model function  
  model <- function(time, stocks, auxs){  
    with(as.list(c(stocks, auxs)),{  
      aBeta <- aEffective.Contact.Rate / aTotalPopulation  
      aLambda <- aBeta * sInfected  
  
      fIR <- sSusceptible * aLambda  
      fRR <- sInfected / aDelay  
  
      dS_dt <- -fIR  
      dI_dt <- fIR - fRR  
      dR_dt <- fRR  
  
      return (list(c(dS_dt,dI_dt,dR_dt),  
                    IR=fIR, RR=fRR,Beta=aBeta,Lambda=aLambda,DEL=aDelay,  
                    CE=aEffective.Contact.Rate,InitI=initInfected))  
    })  
  }  
}
```

The Code (2/3)

```
# setup the individual simulation run
START<-0; FINISH<-20; STEP<-0.01;
simtime <- seq(START, FINISH, by=STEP)

init<-rvec[["initInfected"]]

a<-c(aTotalPopulation=10000,rvec["aEffective.Contact.Rate"],
     rvec["aDelay"],rvec["initInfected"])

stocks  <- c(sSusceptible=10000-init,sInfected=init,sRecovered=0)

o<-data.frame(ode(y=stocks, simtime, func = model,
                  parms=a, method="euler"))
o$RunNumber<-rvec["RunNo"]
o
}
```


The Code (3/3)

```
CE.MIN<-0;          CE.MAX<-7.0
DEL.MIN<-1.0;       DEL.MAX<-10.0
INIT.INF.MIN<-1.0;  INIT.INF.MAX<-25.0;

parRange<-data.frame(
  min=c(CE.MIN, DEL.MIN, INIT.INF.MIN),
  max=c(CE.MAX, DEL.MAX, INIT.INF.MAX)
)

rownames(parRange)<-c("aEffective.Contact.Rate", "aDelay", "initInfected")

NRUNS<-10
p<-data.frame(RunNo=1:NRUNS, Latinhyper(parRange, NRUNS))

out<-apply(p, 1, function(x) runsim(x))

df<-rbind.fill(out)
```

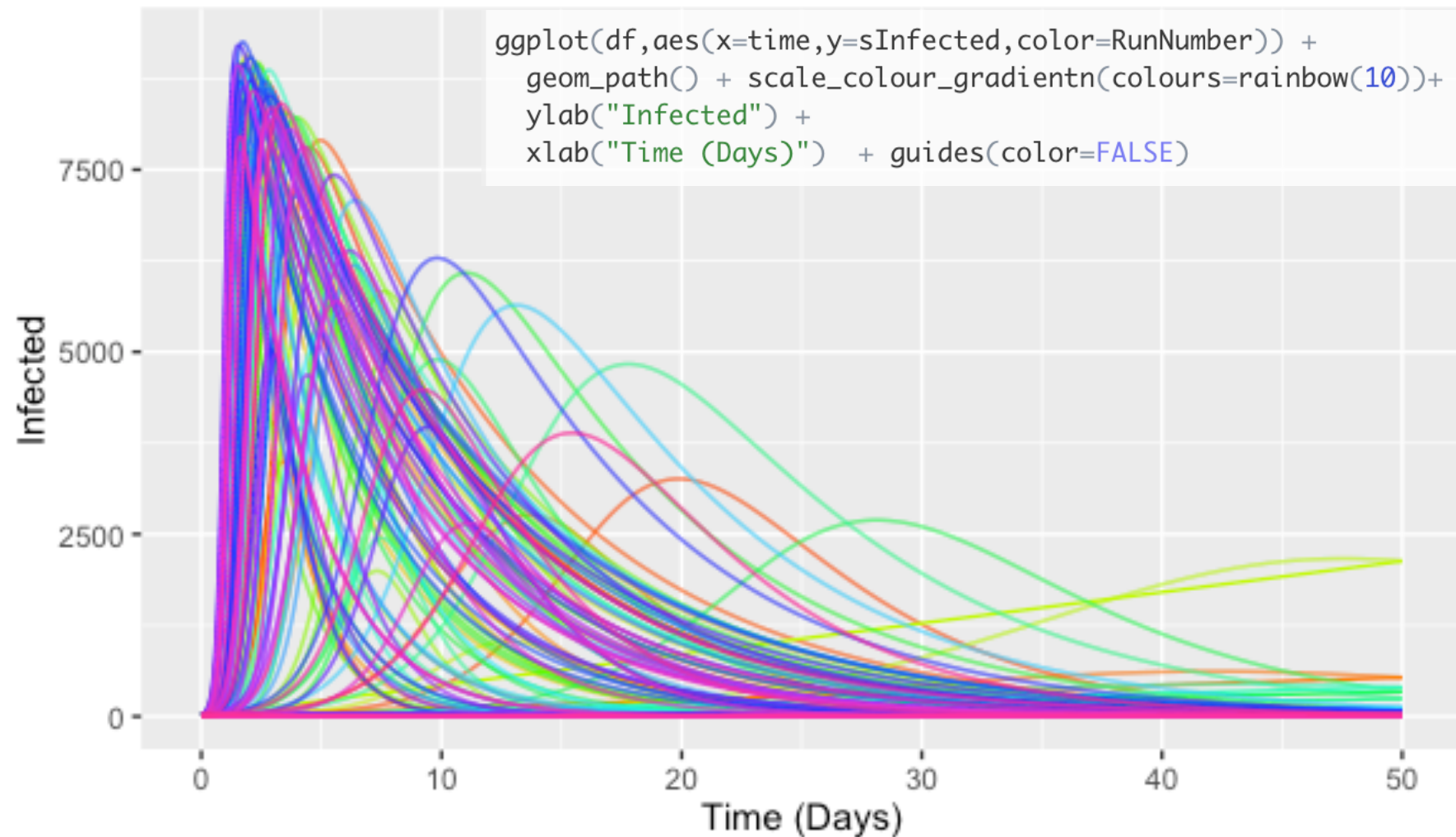
Initial output is a list of data frames: One for each simulation

```
> str(out[[1]])  
'data.frame': 5001 obs. of 12 variables:  
 $ time      : num  0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 ...  
 $ sSusceptible: num  9991 9991 9991 9990 9990 ...  
 $ sInfected   : num   8.65 8.99 9.34 9.71 10.09 ...  
 $ sRecovered  : num   0 0.0103 0.021 0.0321 0.0436 ...  
 $ IR          : num  35.1 36.4 37.9 39.4 40.9 ...  
 $ RR          : num   1.03 1.07 1.11 1.15 1.2 ...  
 $ Beta        : num  0.000406 0.000406 0.000406 0.000406 0.000406 ...  
 $ Lambda      : num  0.00351 0.00365 0.00379 0.00394 0.00409 ...  
 $ DEL         : num   8.41 8.41 8.41 8.41 8.41 ...  
 $ CE          : num   4.06 4.06 4.06 4.06 4.06 ...  
 $ InitI       : num   8.65 8.65 8.65 8.65 8.65 ...  
 $ RunNumber   : num   1 1 1 1 1 1 1 1 1 1 ...
```

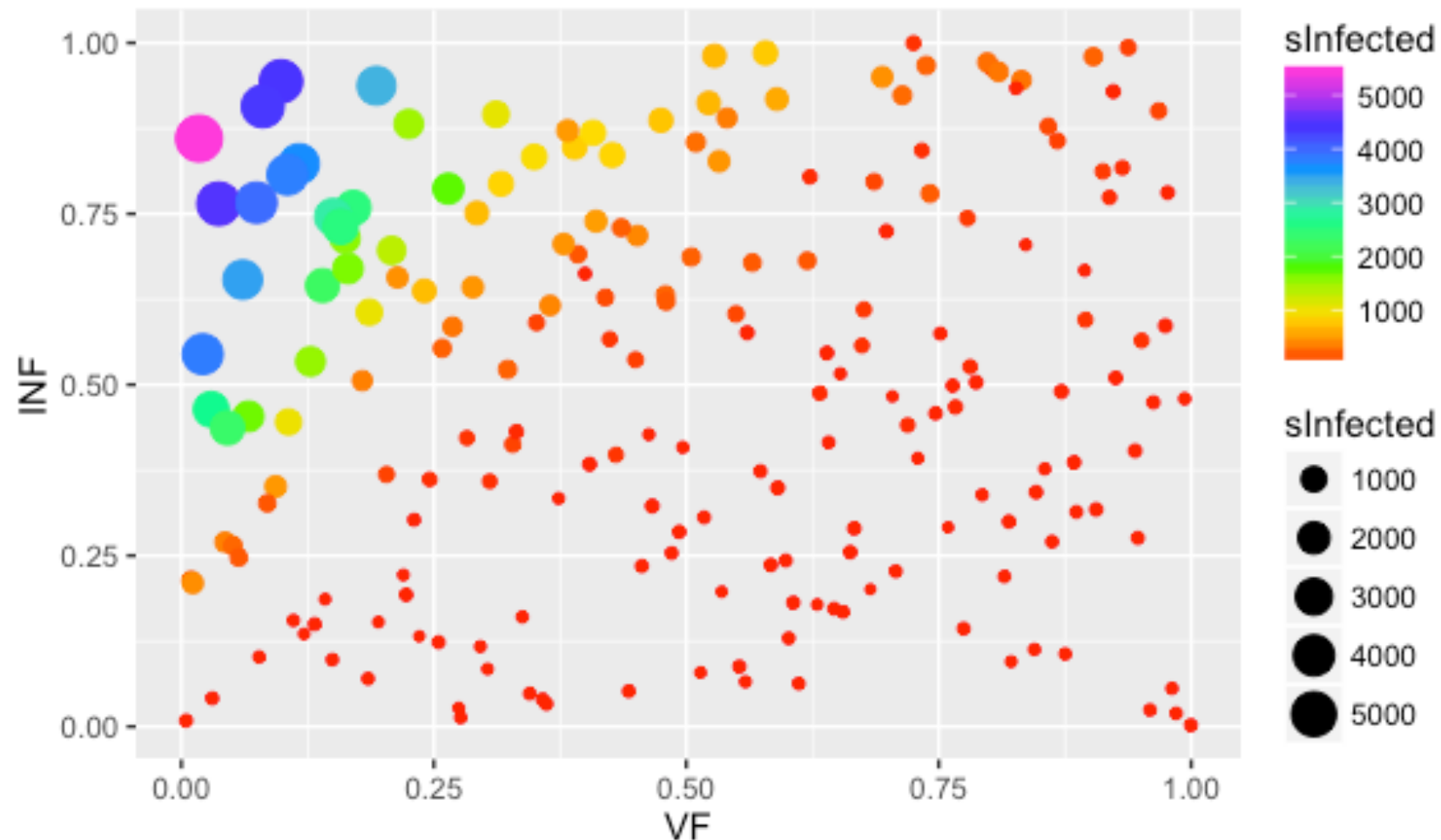
Converted to a single data frame

```
> df<-rbind.fill(out)
>
>
> str(df)
'data.frame': 500100 obs. of 12 variables:
 $ time      : num  0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 ...
 $ sSusceptible: num  9991 9991 9991 9990 9990 ...
 $ sInfected   : num  8.65 8.99 9.34 9.71 10.09 ...
 $ sRecovered  : num  0 0.0103 0.021 0.0321 0.0436 ...
 $ IR          : num  35.1 36.4 37.9 39.4 40.9 ...
 $ RR          : num  1.03 1.07 1.11 1.15 1.2 ...
 $ Beta        : num  0.000406 0.000406 0.000406 0.000406 0.000406 ...
 $ Lambda      : num  0.00351 0.00365 0.00379 0.00394 0.00409 ...
 $ DEL         : num  8.41 8.41 8.41 8.41 8.41 ...
 $ CE          : num  4.06 4.06 4.06 4.06 4.06 ...
 $ InitI       : num  8.65 8.65 8.65 8.65 8.65 ...
 $ RunNumber   : num  1 1 1 1 1 1 1 1 1 1 ...
```

Visualise Simulations



Assignment 2: Exploratory Model Analysis



Assignment Information

- Basic SIR Model ($N = 10000$, Delay = 2)
- Need to add a vaccination flow, and a vaccination fraction $[0,1]$ controlling the flow (no new stocks needed)
- Effective contact rate divided into two elements
 - Contact Rate = 4
 - Infectivity $[0,1]$ probability of passing on infection given contact
 - Effective Contact = Contact Rate * Infectivity
- Run sensitivity for 1000 runs and plot **VF v INF** for **Peak Infected Value** in simulation run.
- `set.seed(1234)`, STEP = 0.01, START = 0, FINISH = 20
- Comment on the results
- Due in Week 1, Semester II.

Sample parameter data (with seed, results should be the same)

```
> parRange
```

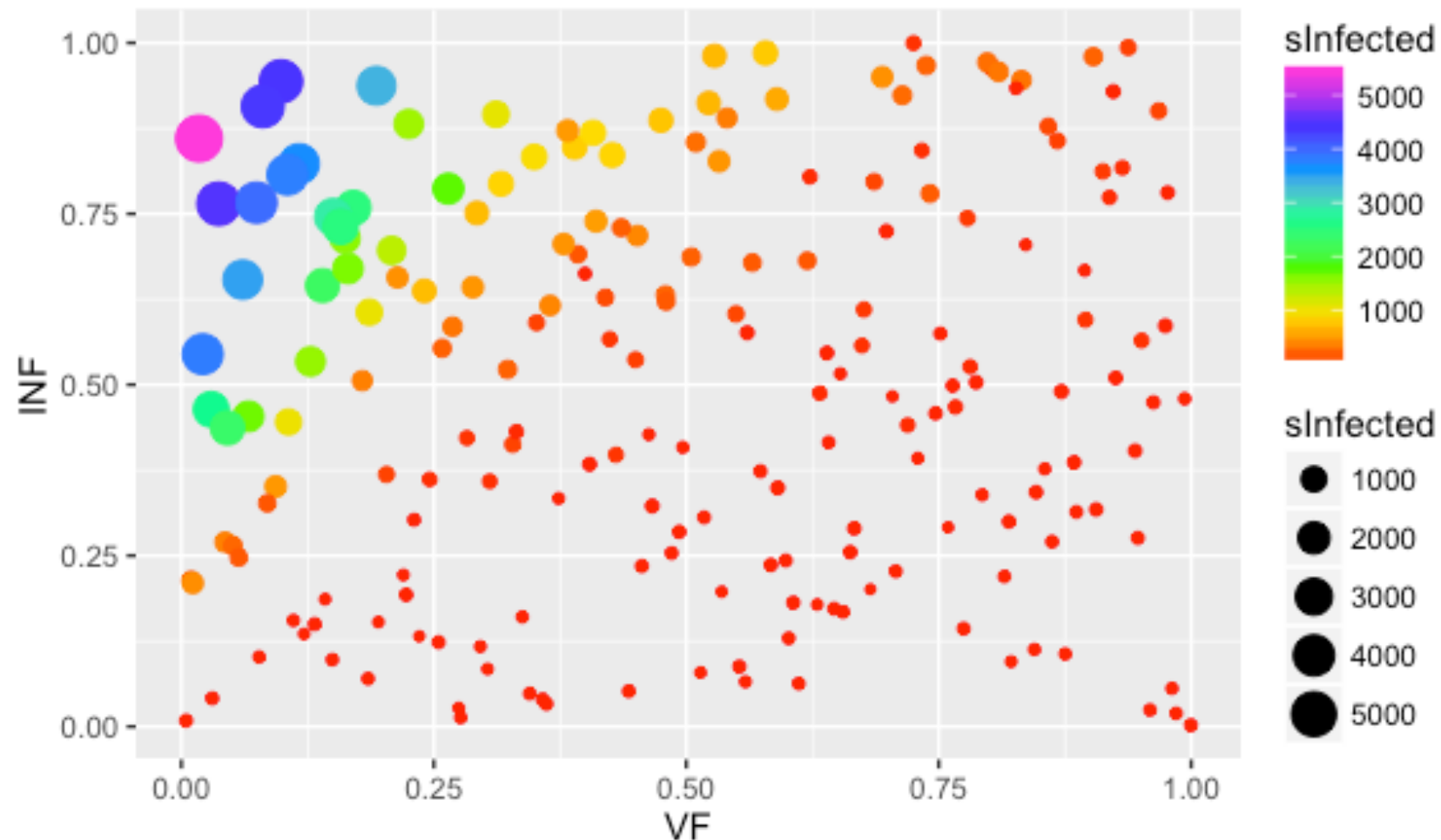
	min	max
aInfectivity	0	1
aVaccFraction	0	1
initInfected	1	25

```
>
```

```
> head(p)
```

	RunNo	aInfectivity	aVaccFraction	initInfected
1	1	0.03330377	0.3614049	24.500516
2	2	0.31764180	0.9058709	21.698496
3	3	0.36158747	0.2458511	11.693240
4	4	0.92883928	0.9228027	4.162164
5	5	0.48763154	0.6321440	16.931328
6	6	0.50366151	0.7869459	13.646760

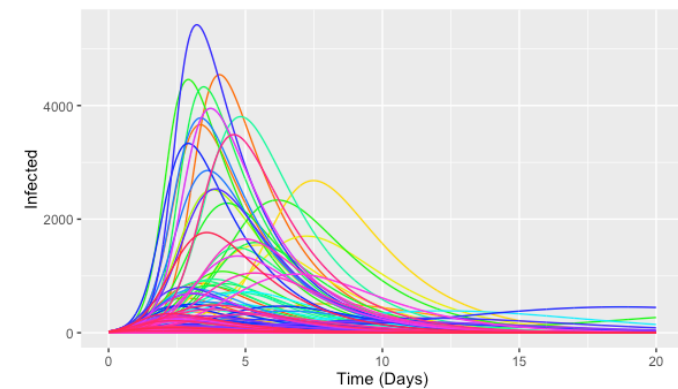
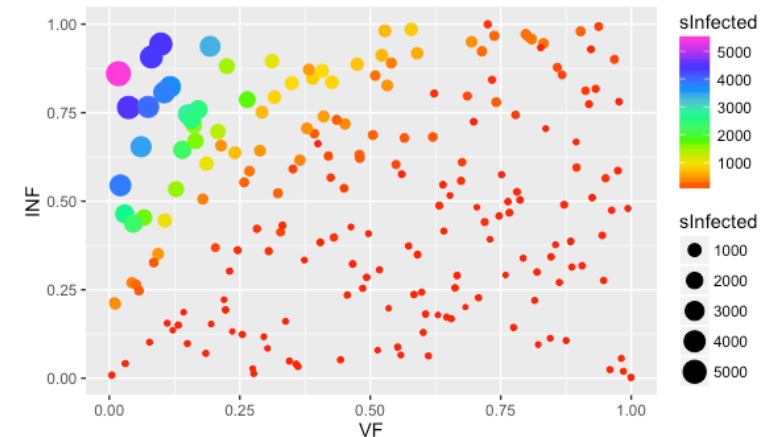
Aim: Produce the following graph
for 200 simulations



Data check (first 10 for max infections)

```
> ans[1:10,]
```

	sInfected	VF	INF
1	24.500516	0.3614049	0.03330377
2	30.314068	0.9058709	0.31764180
3	61.094769	0.2458511	0.36158747
4	44.231923	0.9228027	0.92883928
5	56.223090	0.6321440	0.48763154
6	38.195783	0.7869459	0.50366151
7	36.882682	0.6392185	0.54653833
8	7.852881	0.2960440	0.11702087
9	19.663710	0.5175471	0.30602201
10	25.002103	0.1319748	0.14992817



Exam Question (A2015) – part(a)

2. (a) Suppose we have a town with 100,000 ($=N$) individuals, of which 1% were infectious with influenza, with $R_0 = 2$ and $D=2$ days (where D is the recovery delay)
- Calculate the force of infection λ
 - Calculate the Herd Immunity Threshold
 - Plot the Herd Immunity Threshold where the values of R_0 range from 1 to 10 (in steps of 1)

(6)

Exam Question (A2015) – part(b)

- (b) Design a stock and flow model (with equations) to simulate the spread of seasonal influenza. Assume that the value for R_0 is 2, and that the average recovery delay is 2 days. The model should have the following features:
- Its core structure should be based on the *Susceptible – Exposed – Infected – Recovered* model.
 - Exposed people are not infectious, but become infectious after a first order delay of 5 days. The inflow into the *Exposed* stock is the *infection rate*.
 - 1% of people who are infected become hospitalised for a period of 10 days, before recovering. This feature must be captured in the stock and flow model.

(8)

Exam Question (A2015) – part(c)

- (c) Show how the model would need to be modified in order to represent different cohorts, for example, males and females in the population, and young, adults and elderly.

(6)