System Dynamics Modeling with R

System Dynamics Collaborative Learning Meeting

Worcester Polytechnic Institute (WPI)

April 27th 2017

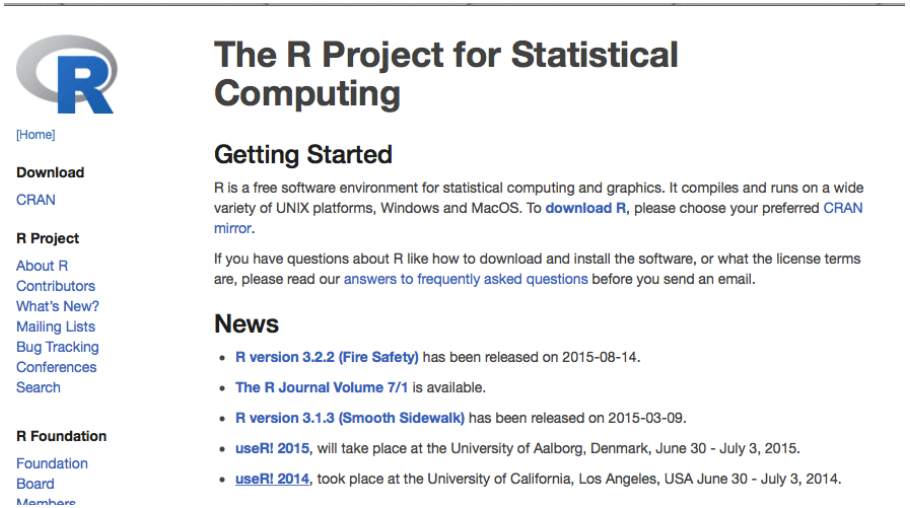
Jim Duggan,
School of Engineering & Informatics
National University of Ireland Galway.

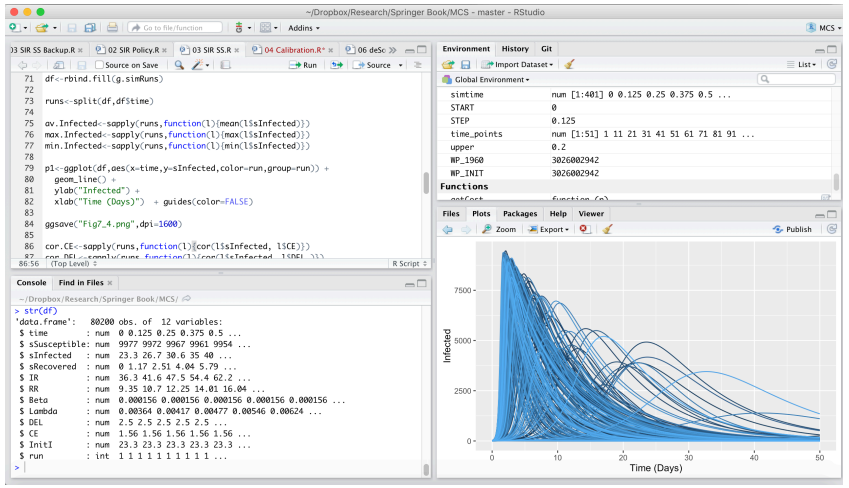
Overview

1. R and Data Science (Overview)
2. System Dynamics Modeling with R
   - Models using deSolve
   - Behaviour Modes
   - Disaggregate Models
   - Sensitivity Runs
   - Statistical Screening

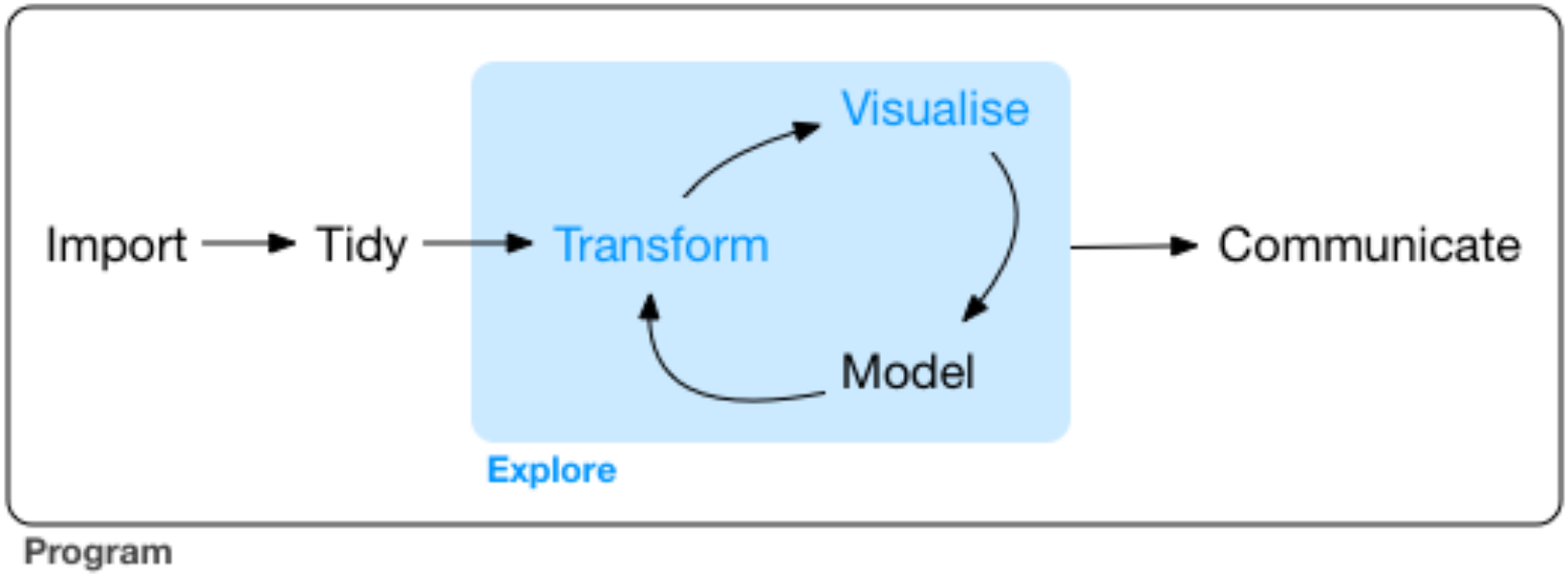
The R Project for Statistical Computing

- R's *mission* is to enable the best and most thorough exploration of data possible (Chambers 2008).
- It is a dialect of the S language, developed at Bell Laboratories
- ACM noted that *S "will forever alter the way people analyze, visualize, and manipulate data"*



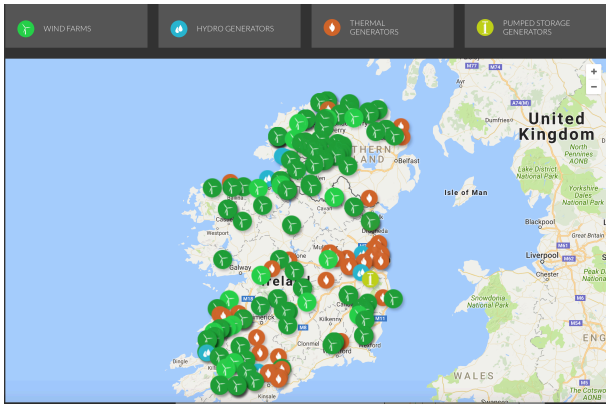


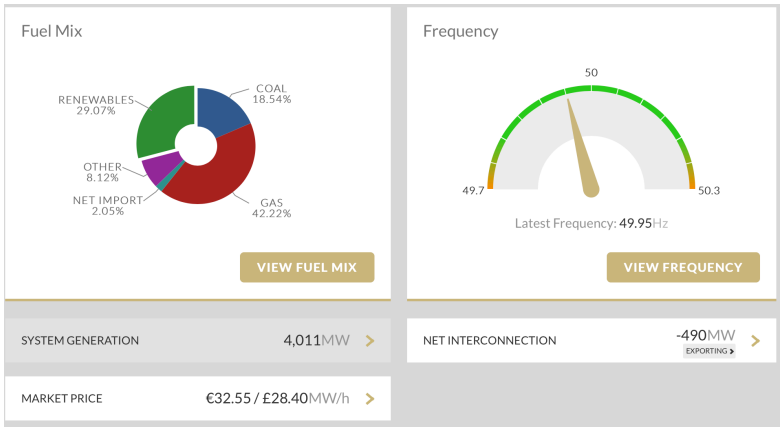
(1) Data Science Process in R



"Data exploration is the art of looking at your data, rapidly generating hypotheses, quickly testing them, then repeating again and again and again." (Wickham and Grolemund 2017).

http://smartgriddashboard.eirgrid.com



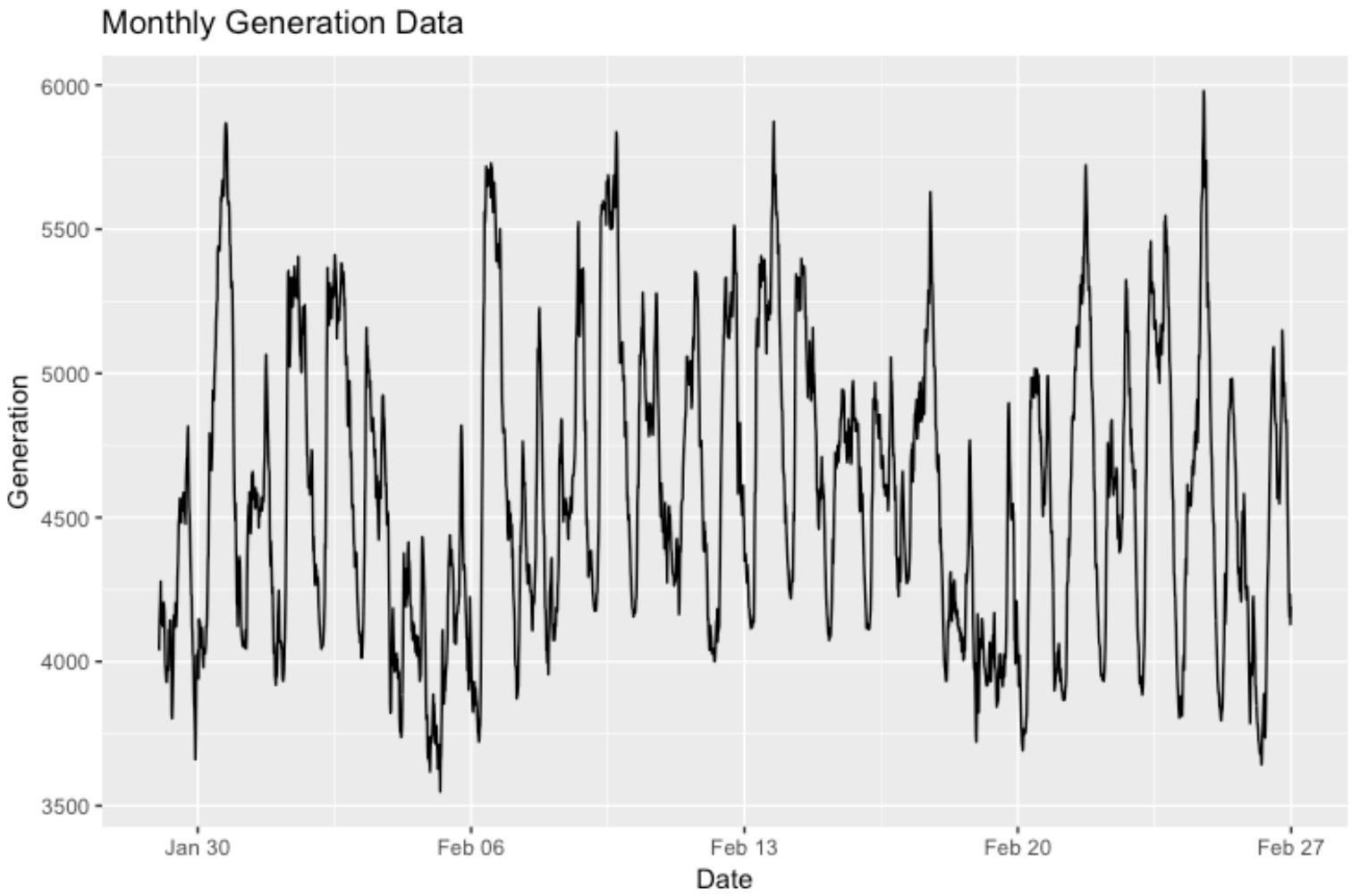



```
> ener
# A tibble: 2,784 × 11
             DateTime Demand Generation  Wind   CO2 NetImports  EWIC Moyle HourOfDay MinuteOfDay DayOfWeek
               <dttm>  <int>      <int> <int> <int>      <int> <int> <int>     <int>       <int>     <ord>
1  2017-01-29 00:00:00   3834       4041   449   552       -145   -33  -112         0           0       Sun
2  2017-01-29 00:15:00   3785       4041   505   548       -200  -108   -92         0          15       Sun
3  2017-01-29 00:30:00   3708       4130   521   544       -294  -183  -111         0          30       Sun
4  2017-01-29 00:45:00   3634       4181   492   543       -419  -258  -161         0          45       Sun
5  2017-01-29 01:00:00   3581       4211   538   555       -503  -333  -170         1           0       Sun
6  2017-01-29 01:15:00   3552       4278   561   531       -598  -379  -219         1          15       Sun
7  2017-01-29 01:30:00   3491       4133   484   545       -516  -374  -142         1          30       Sun
8  2017-01-29 01:45:00   3435       4143   474   551       -581  -365  -216         1          45       Sun
9  2017-01-29 02:00:00   3374       4158   442   550       -653  -373  -280         2           0       Sun
10 2017-01-29 02:15:00   3329       4135   421   550       -676  -377  -299         2          15       Sun
# ... with 2,774 more rows
```

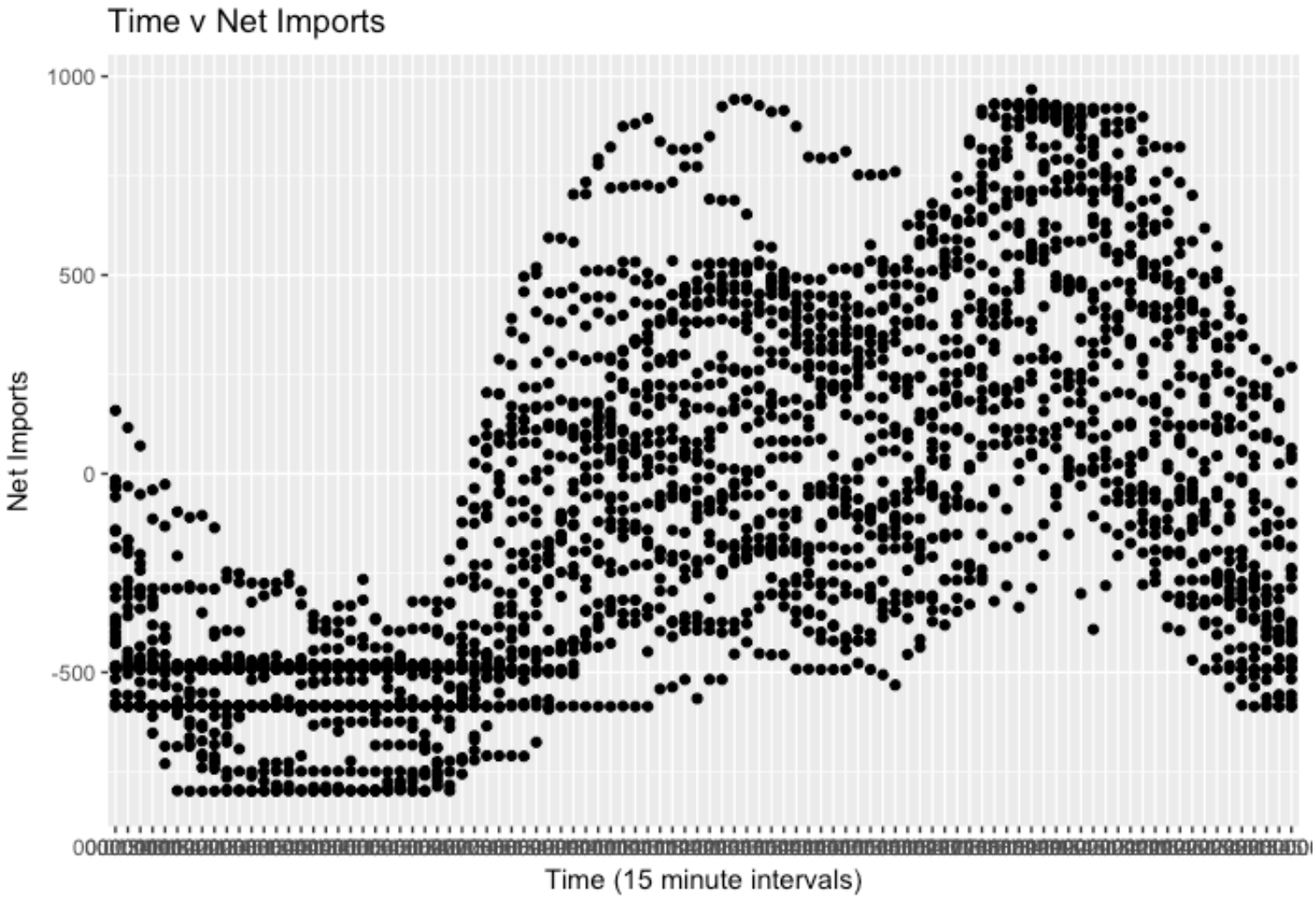
Exploring Data Relationships

- Time series:
  - Generation data over the entire month
  - Generation data over a day
- Time of Day v Net Imports
- Demand v Net Imports
- Wind Generation v CO2 Emissions
- Comparing Wind Generation with Overall Generation

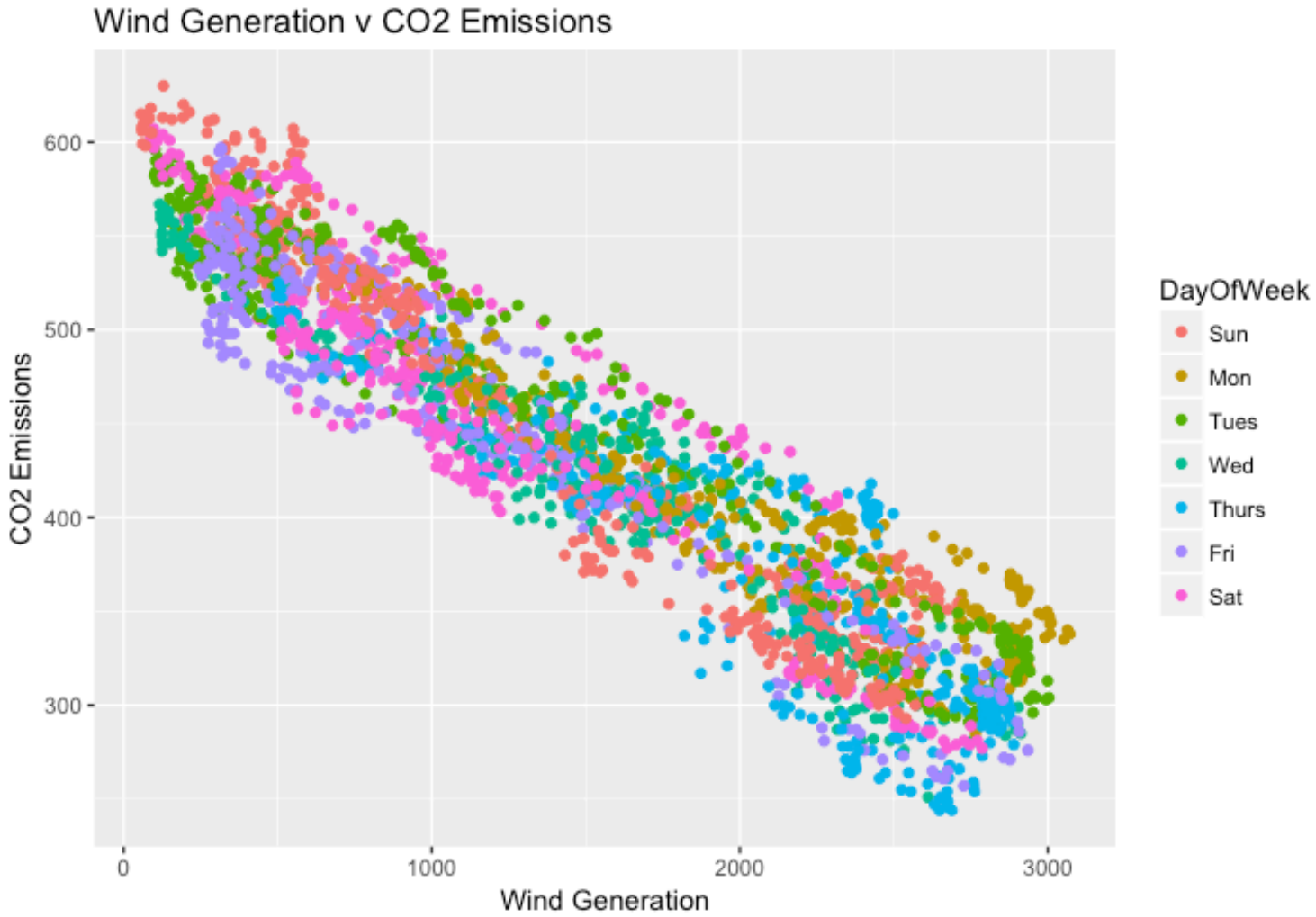
```
ggplot(data = ener) +
  geom_line(mapping = aes(x=DateTime,y=Generation)) +
  xlab("Date") + ylab("Generation") + ggtitle("Monthly Generation Data")
```



```
ggplot(data = ener) +
  geom_point(mapping = aes(x=as.factor(Time),y=NetImports)) +
  xlab("Time (15 minute intervals)") + ylab("Net Imports") +
  ggtitle("Time v Net Imports")
```



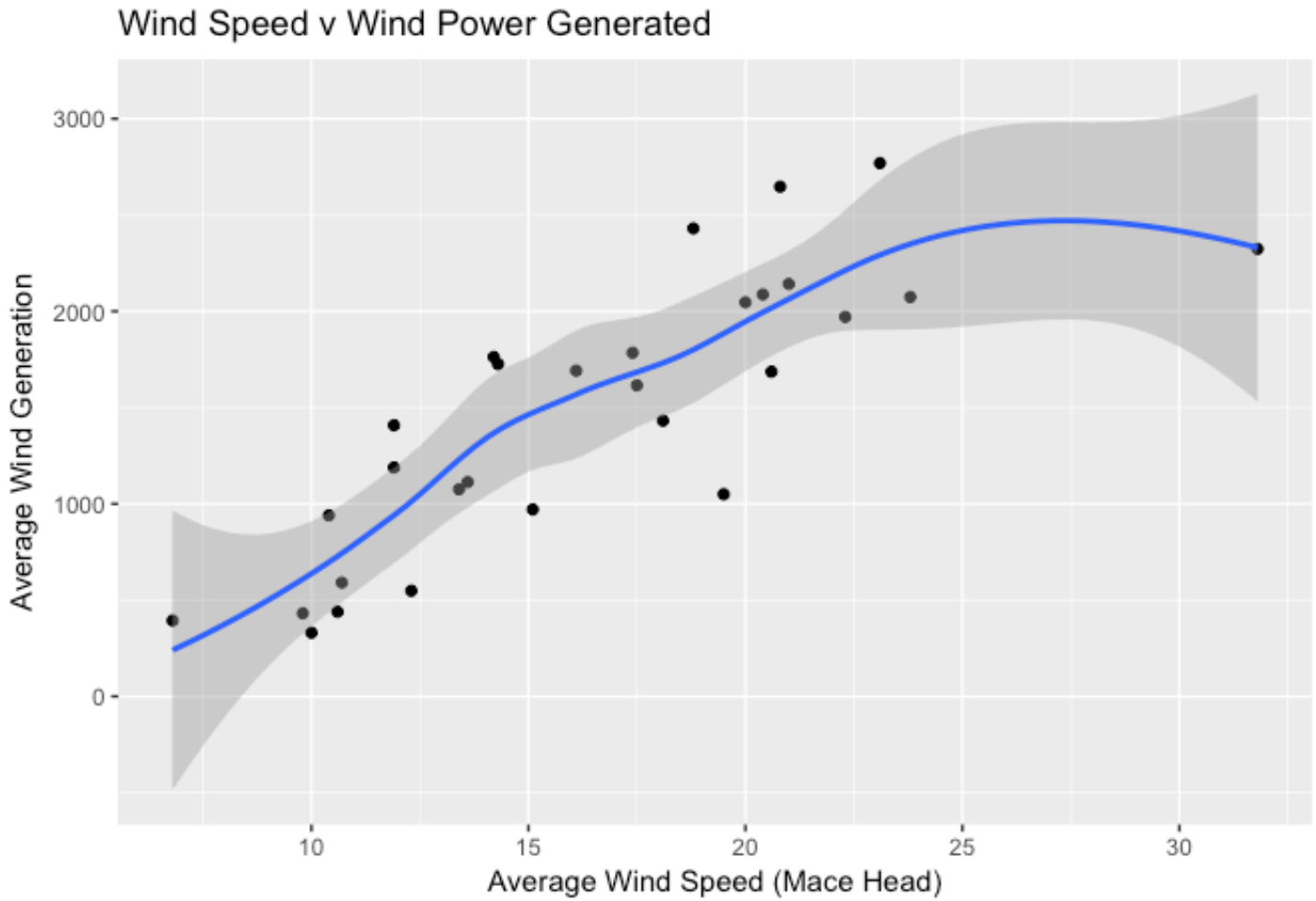
```
ggplot(data = ener) +
  geom_point(mapping = aes(x=Wind,y=CO2,colour=DayOfWeek)) +
  xlab("Wind Generation") + ylab("CO2 Emissions") +
  ggtitle("Wind Generation v CO2 Emissions")
```



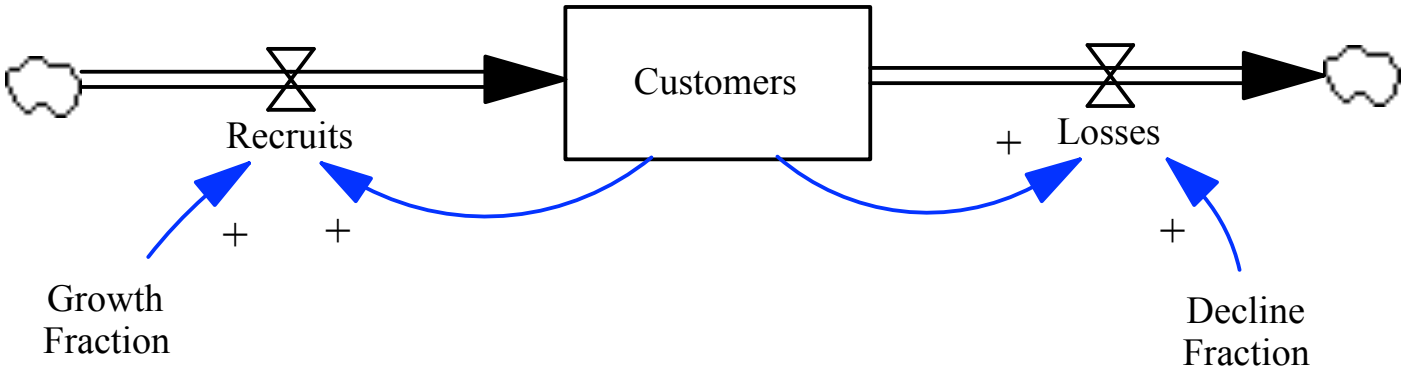
Joining Data Sets

```
> ener[1:5,]
# A tibble: 5 × 13
             DateTime       Date     Time Demand Generation  Wind   CO2 NetImports  EWIC Moyle
               <dttm>      <chr>    <chr>  <int>      <int> <int> <int>      <int> <int> <int>
1 2017-01-29 00:00:00 2017-01-29 00:00:00   3834       4041   449   552       -145   -33  -112
2 2017-01-29 00:15:00 2017-01-29 00:15:00   3785       4041   505   548       -200  -108   -92
3 2017-01-29 00:30:00 2017-01-29 00:30:00   3708       4130   521   544       -294  -183  -111
4 2017-01-29 00:45:00 2017-01-29 00:45:00   3634       4181   492   543       -419  -258  -161
5 2017-01-29 01:00:00 2017-01-29 01:00:00   3581       4211   538   555       -503  -333  -170
# ... with 3 more variables: HourOfDay <int>, MinuteOfDay <int>, DayOfWeek <ord>
>
>
> weather[1:5,]
# A tibble: 5 × 7
        Date Rainfall MaxTemp MinTemp GrassMinTemp AVRWind MaxWindGust
      <date>    <dbl>   <dbl>   <dbl>        <dbl>   <dbl>       <int>
1 2017-01-27      7.9     8.7     4.3         -0.7    11.6          NA
2 2017-01-28      3.5     8.0     4.5          2.9    12.6          NA
3 2017-01-29      4.7     9.0     4.9          3.7     9.8          NA
4 2017-01-30      7.8    11.2     7.1          5.8    14.3          NA
5 2017-01-31      0.0    10.3     7.3          5.8    10.0          NA
```

```
ggplot(data = gen_weather,mapping = aes(x=AVRWind,y=AverageWindGeneration)) +
  geom_point() +
  geom_smooth()+
  xlab("Average Wind Speed (Mace Head)") + ylab("Average Wind Generation") +
  ggtitle("Wind Speed v Wind Power Generated")
```



(2.1) Simple Customer Model



$$Customers = INTEGRAL(Recruits - Losses, 10000)$$

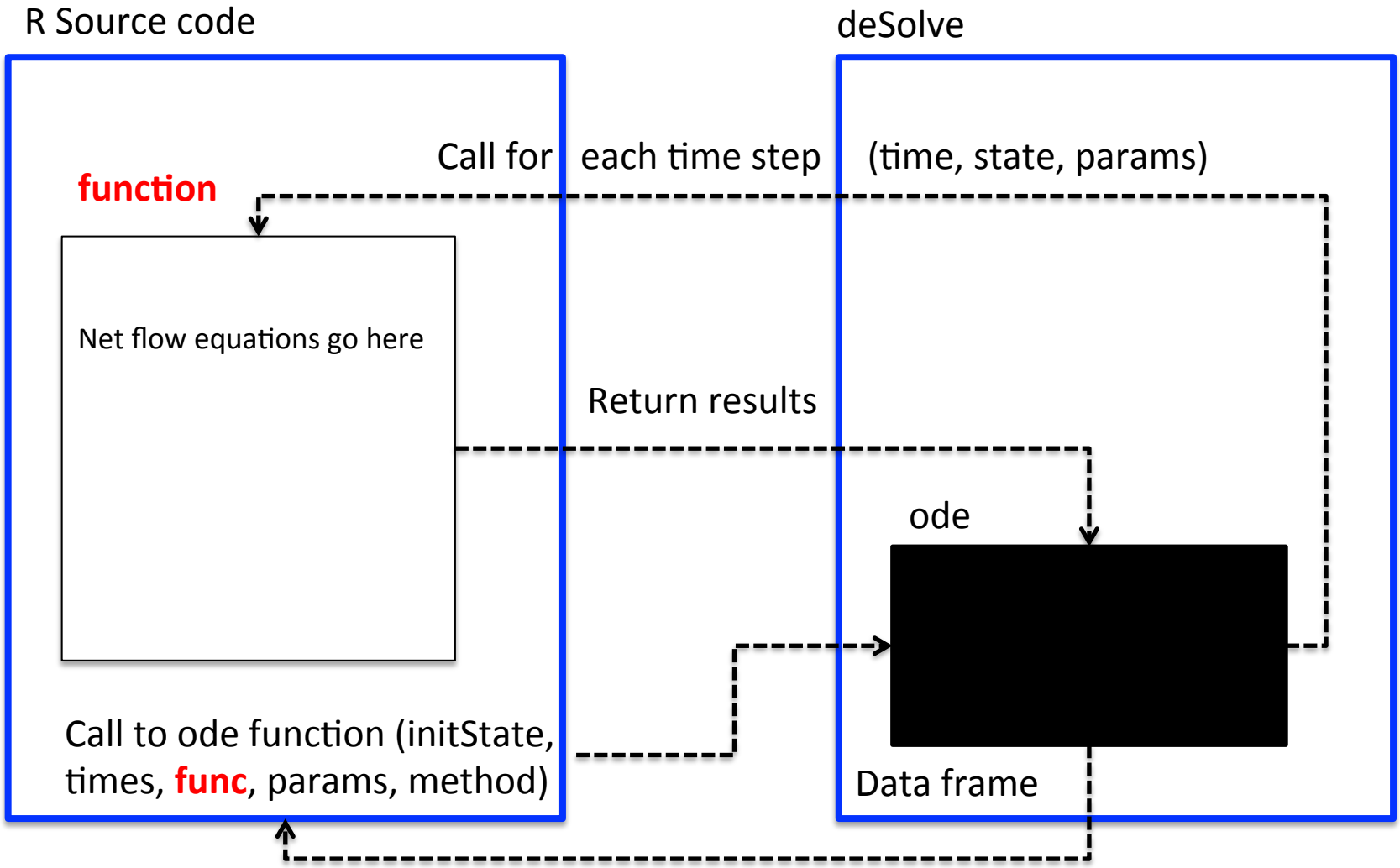
$$Recruits = Customers \times Growth\ Fraction$$

$$Losses = Customers \times Decline\ Fraction$$

$$Growth\ Fraction = 0.07$$

$$Decline\ Fraction = 0.03$$

deSolve Approach (callbacks)



Model File in R

```
library(deSolve)
library(ggplot2)
library(scales)

# Setup simulation times and time step
START<-2015; FINISH<-2030; STEP<-0.5

# Create time vector
simtime <- seq(START, FINISH, by=STEP)

# Create stock and auxs
stocks  <- c(sCustomers=10000)
auxs    <- c(aGrowthFraction=0.08, aDeclineFraction=0.03)
```

Model in a function

```
model <- function(time, stocks, auxs){
  with(as.list(c(stocks, auxs)),{

    fRecruits<-sCustomers*aGrowthFraction

    fLosses<-sCustomers*aDeclineFraction

    dC_dt <- fRecruits - fLosses

    ans<-list(c(dC_dt),
              Recruits=fRecruits, Losses=fLosses,NetFlow=dC_dt,
              GF=aGrowthFraction,DF=aDeclineFraction)

    return (ans)
  })
}
```

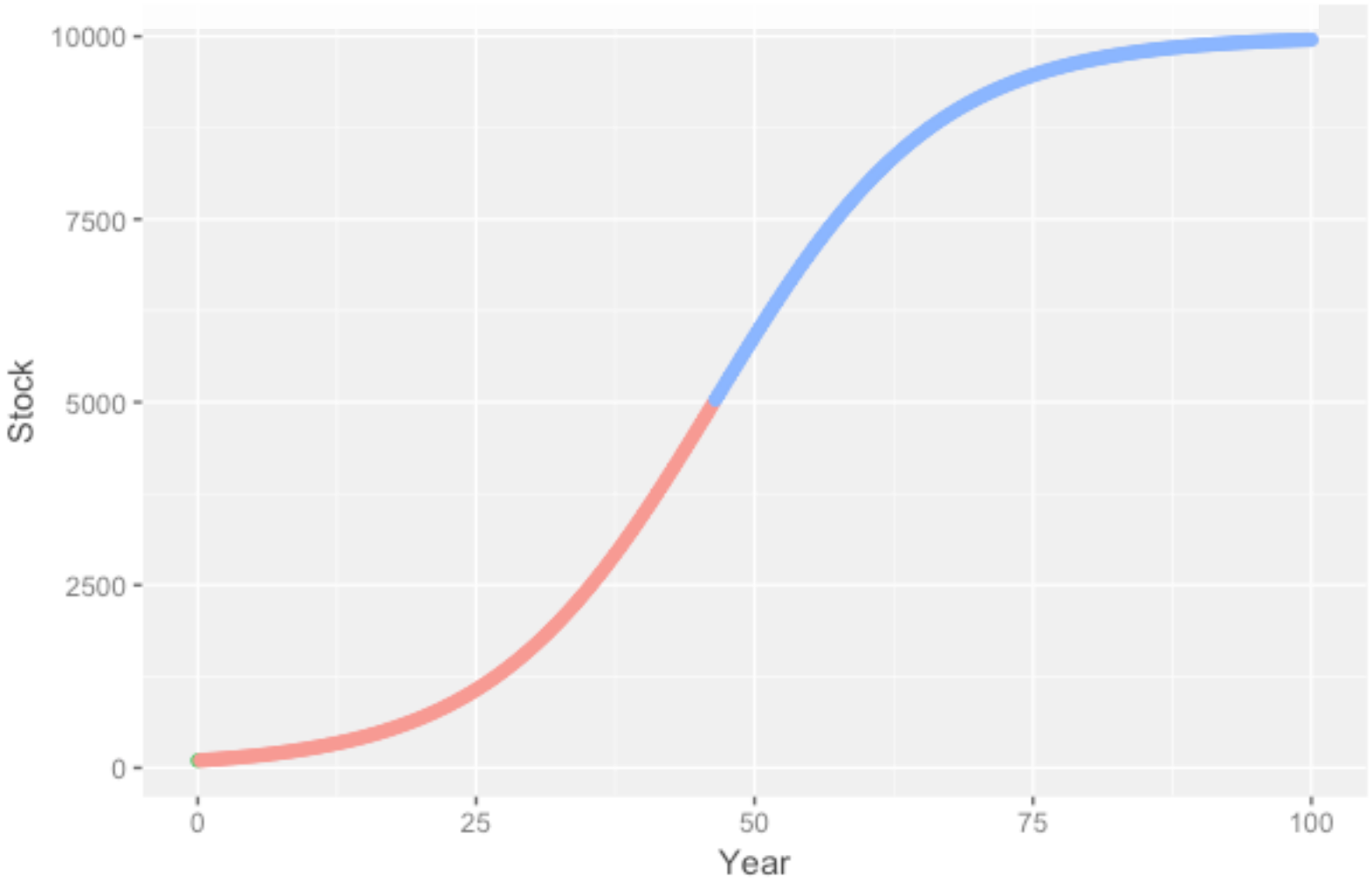
Run Simulation

```
# Run simulation
o<-data.frame(ode(y=stocks, times=simtime, func = model,
                  parms=auxs, method='euler'))

qplot(x=time,y=sCustomers,data=o) + geom_line()


# Plots and output
p1<-ggplot()+
  geom_line(data=o,aes(time,o$sCustomers,color="red"))+
  scale_y_continuous(labels = comma)+
  ylab("Customers")+
  xlab("Year") +
  theme(legend.position="none")
```

(2.2) Behaviour Modes

```
derivn<-function(voi,time){
  c(0.0,diff(voi)/diff(time))
}

abm<-function(v){
  ifelse(v==0.0,"LIN",
         ifelse(v<0,"LOG","EXP"))
}
```

```
o$abm<-derivn(abs(o$NetFlow),o$time)

o$bmode<-abm(o$abm)
```



(2.3) Disaggregate Models

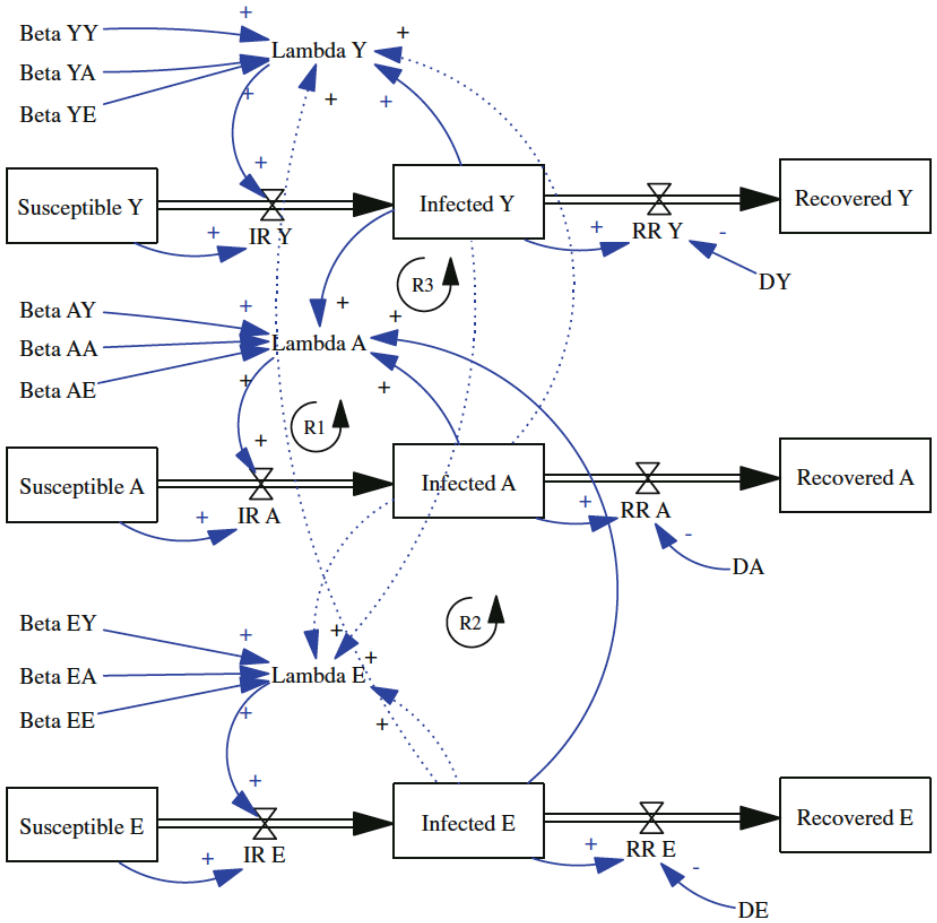
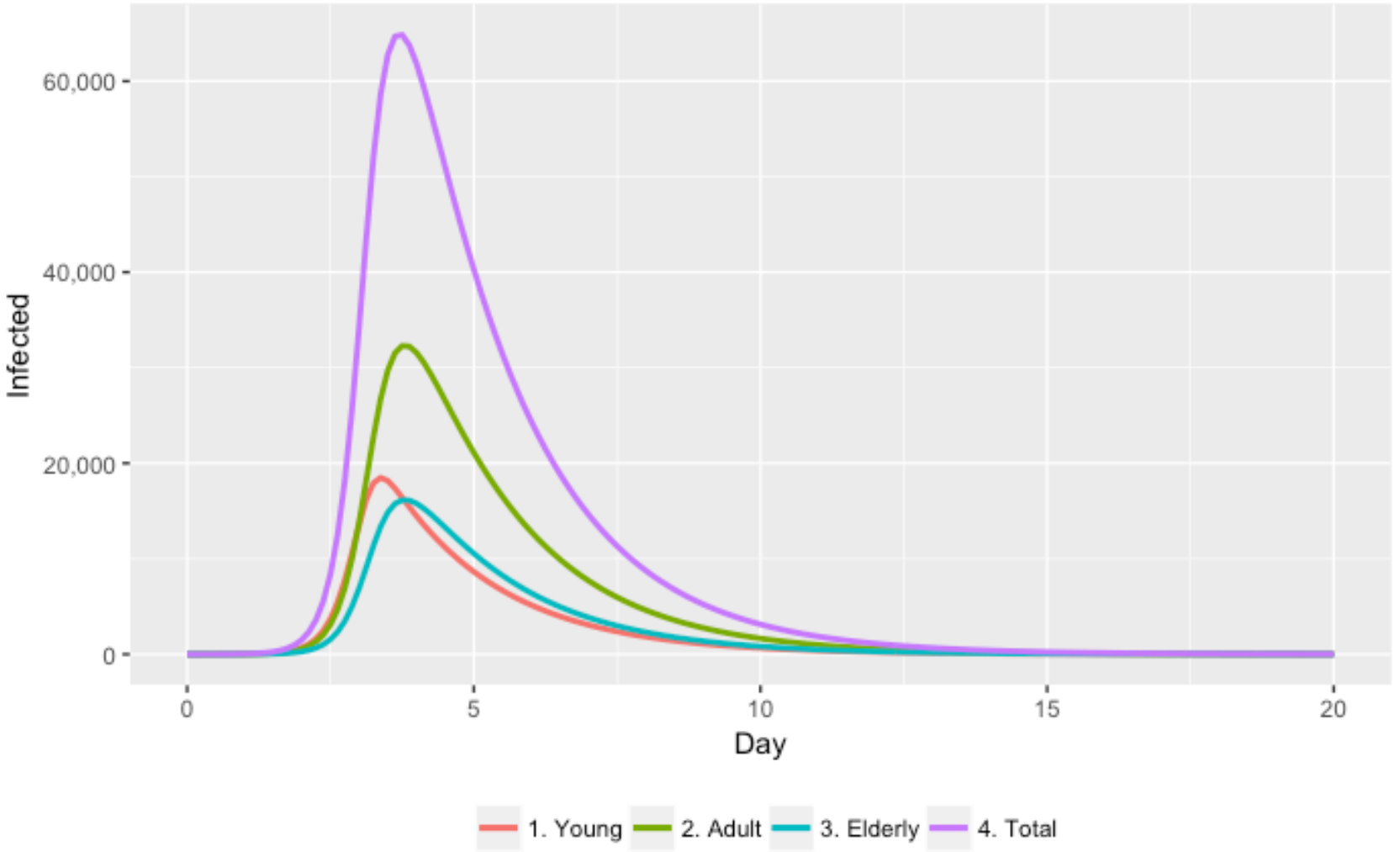


Fig. 5.5 A disaggregated SIR model (three cohorts)

```
model <- function(time, stocks, auxs){
  with(as.list(c(stocks, auxs)),{
    #convert the stocks vector to a matri
    states<-matrix(stocks,nrow=NUM_COHORTS

    Susceptible <- states[,1]
    Infected    <- states[,2]
    Recovered   <- states[,3]

    Lambda      <- beta %*% Infected

    IR          <- Lambda * Susceptible
    RR          <- Infected / delays

    dS_dt  <- -IR
```

Epi-Curve Output



(2.4) 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.

Author Karline Soetaert <karline.soetaert@nioz.nl>, Thomas Petzoldt <thomas.petzoldt@tu-dresden.de>

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

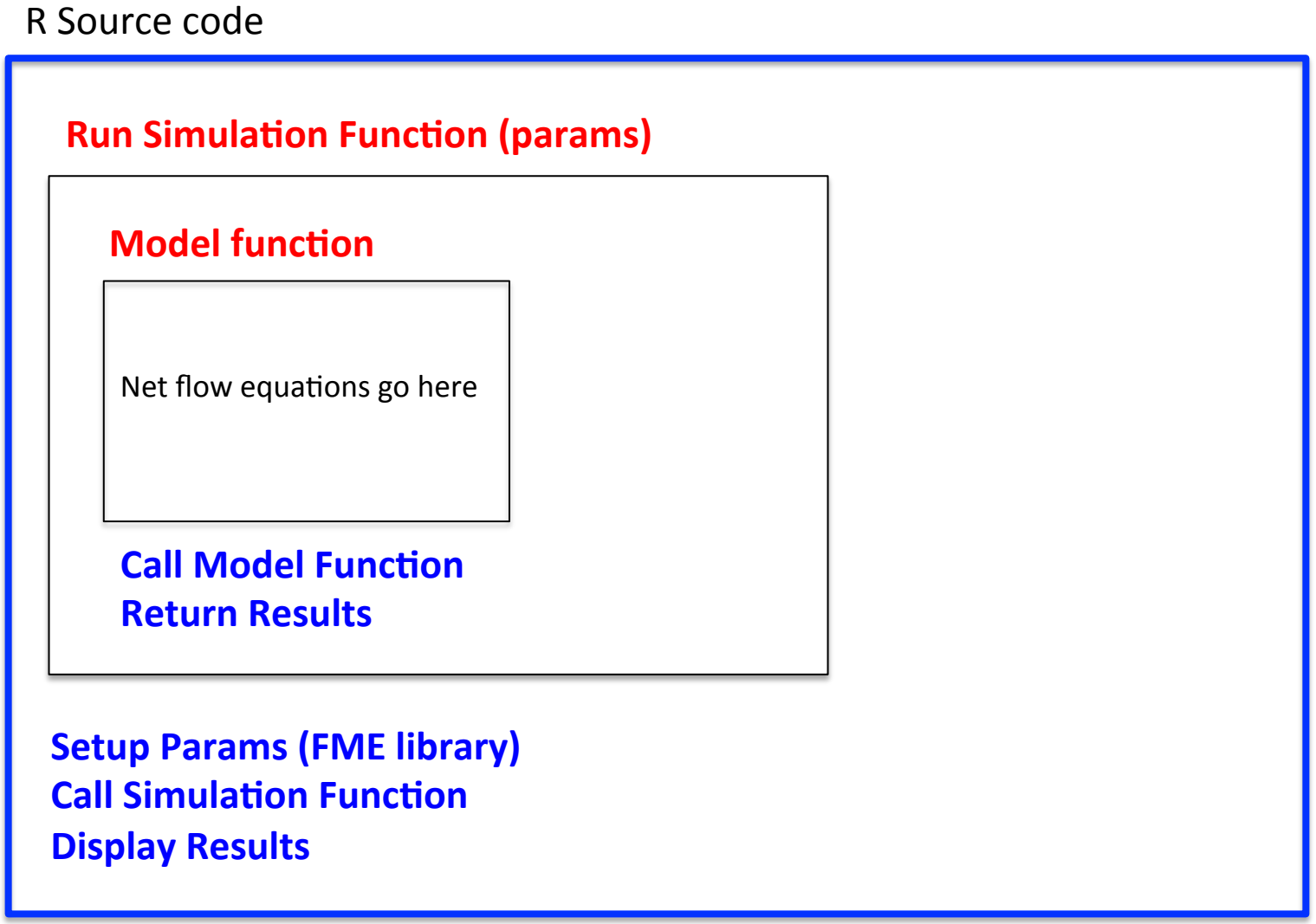
Depends R (>= 2.6), deSolve, rootSolve, coda

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



Generating Parameters

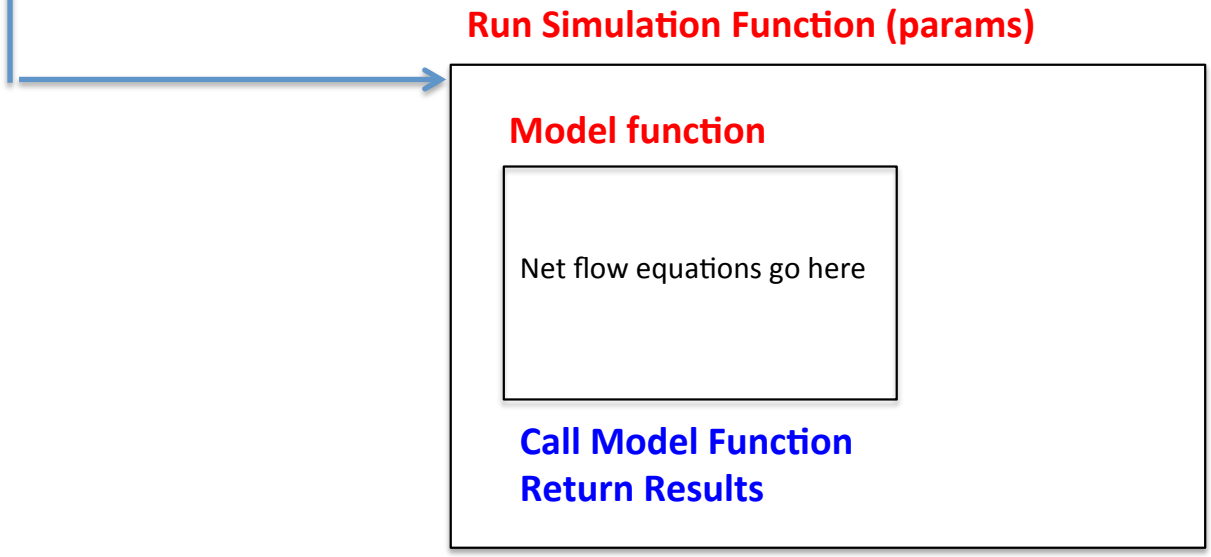
```
CE.MIN<-0;            CE.MAX<-7.0
DEL.MIN<-1.0;         DEL.MAX<-10.0
INIT.INF.MIN<-1.0;    INIT.INF.MAX<-25.0;

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
```



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)
```

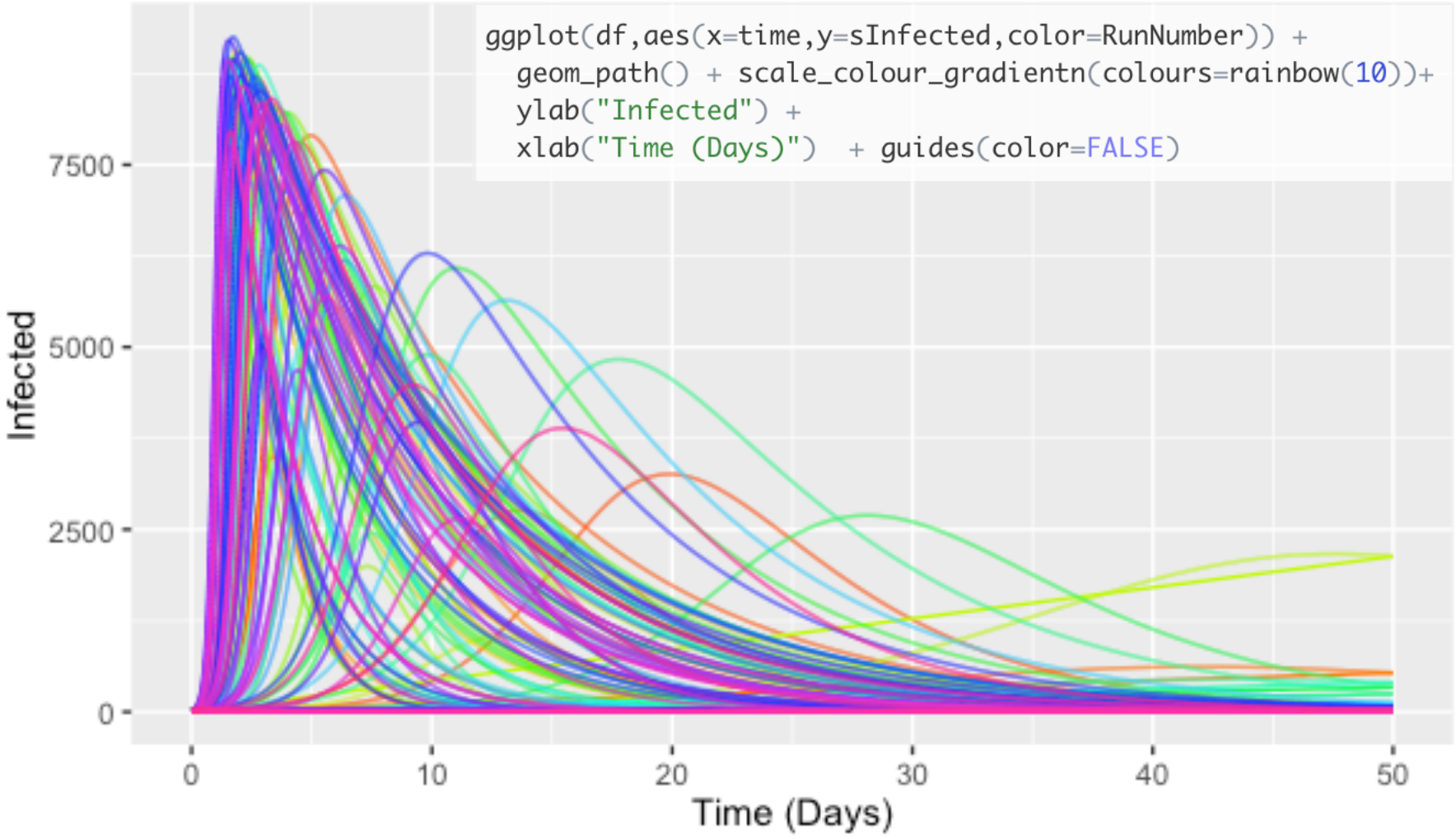
Initial output is a list of data frames: One for each simulation

```
> 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 ...
```

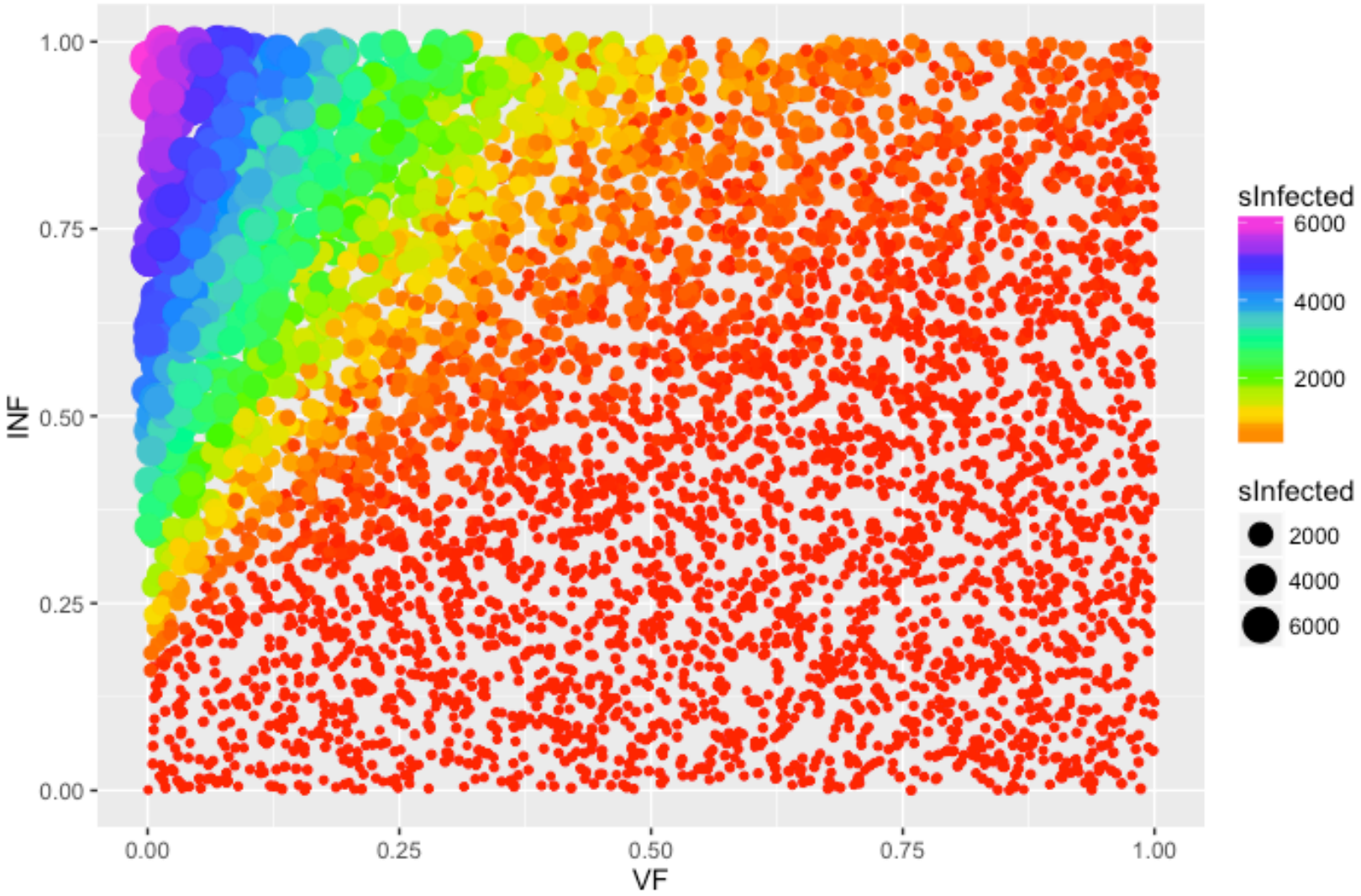
Converted to a single data frame

```
> 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



N = 5000


1.00
0.75
0.50
0.25
0.00
INF
0.00
0.25
0.50
0.75
1.00
VF
sInfected
6000
4000
2000
sInfected
2000
4000
6000

(2.5) Statistical Screening

The system dynamics approach leads to models with a large number of highly uncertain parameters, so we should ask ourselves which of the parameters are really important. Ford and Flynn (2005)

Statistical screening utilizes the sensitivity output data to calculate the *correlation coefficients* between parameters and a user-defined system performance variable (Taylor, Ford and Ford 2010).

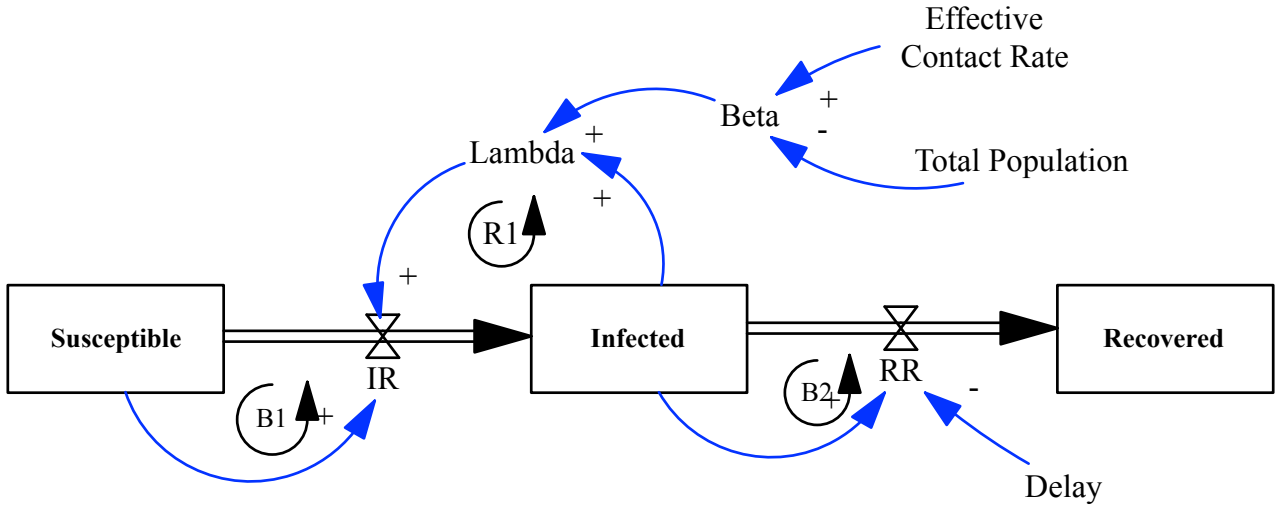
$$r = \frac{\sum (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum (X_i - \bar{X})^2 \sum (Y_i - \bar{Y})^2}}$$

Steps (based on Taylor et al. 2010)

1. **Select a set of exogenous model parameters, and a system performance variable for analysis. Select appropriate parameter ranges.**
2. **Calculate the correlation coefficients between the selected exogenous model parameters and the system performance variables. Plot the correlation coefficients and the behavior of the performance variable over time.**
3. Select the time interval for analysis, by examining the time series data of both the performance variable, and the correlation coefficients.
4. Generate a list of high-leverage parameters, which are those that recorded the highest absolute correlation coefficient values during the selected time period.
5. Based on the parameters selected from step 4, identify the high-leverage model structure(s) that are directly influenced by the parameters..
6. Develop explanations about how each parameter (or set of parameters), and the model structures they influence, drive the overall system behavior.

Model - SIR

Parameter	Description	Min	Max
$Infected_{INIT}$	The initial value of number infected in the model. A number greater than zero is required in order for the disease to spread.	1.0	25.0
C_E	Effective contact rate, where higher values increase the spread of a disease.	0	7.0
D	Recovery delay, where a longer delay will result in people spending longer times in the infected stock.	1.0	10.0



N=200, 40200 Observations

```
> round(head(df),2)
  time sSusceptible sInfected sRecovered     IR   RR Beta Lambda  DEL   CE InitI run
1 0.00      9995.99      4.01       0.00  18.63 0.96    0   0.00 4.16 4.65  4.01   1
2 0.12      9993.66      6.22       0.12  28.87 1.50    0   0.00 4.16 4.65  4.01   1
3 0.25      9990.05      9.64       0.31  44.74 2.32    0   0.00 4.16 4.65  4.01   1
4 0.38      9984.46     14.94       0.60  69.31 3.59    0   0.01 4.16 4.65  4.01   1
5 0.50      9975.80     23.16       1.05 107.32 5.57    0   0.01 4.16 4.65  4.01   1
6 0.62      9962.38     35.88       1.74 166.03 8.63    0   0.02 4.16 4.65  4.01   1
> round(tail(df),2)
       time sSusceptible sInfected sRecovered IR    RR Beta Lambda  DEL   CE InitI run
40195 24.38           0    139.65    9860.35  0 25.94    0   0.08 5.38 5.93   6.7 200
40196 24.50           0    136.41    9863.59  0 25.34    0   0.08 5.38 5.93   6.7 200
40197 24.62           0    133.25    9866.75  0 24.75    0   0.08 5.38 5.93   6.7 200
40198 24.75           0    130.15    9869.85  0 24.17    0   0.08 5.38 5.93   6.7 200
40199 24.88           0    127.13    9872.87  0 23.61    0   0.08 5.38 5.93   6.7 200
40200 25.00           0    124.18    9875.82  0 23.06    0   0.07 5.38 5.93   6.7 200
```

Challenge: Need to group the data by time step for correlation analysis

split(x,f)

Arguments

- x vector or data frame containing values to be divided into groups.
- f a 'factor' in the sense that as.factor(f) defines the grouping, or a list of such factors in which case their interaction is used for the grouping.

Split the data set

```
> runs<-split(df,df$time)
> round(head(runs[[1]]),2)
     time sSusceptible sInfected sRecovered     IR   RR Beta Lambda  DEL   CE InitI run
1       0      9995.99      4.01          0  18.63 0.96    0   0.00 4.16 4.65  4.01   1
202     0      9997.29      2.71          0  15.17 0.38    0   0.00 7.20 5.61  2.71   2
403     0      9981.98     18.02          0 102.64 2.76    0   0.01 6.54 5.71 18.02   3
604     0      9977.28     22.72          0  96.75 5.68    0   0.01 4.00 4.27 22.72   4
805     0      9995.46      4.54          0   3.88 1.51    0   0.00 3.00 0.86  4.54   5
1006    0      9989.73     10.27          0  57.92 7.96    0   0.01 1.29 5.65 10.27   6
> round(head(runs[[2]]),2)
     time sSusceptible sInfected sRecovered     IR    RR Beta Lambda  DEL   CE InitI run
2    0.12      9993.66      6.22       0.12  28.87  1.50    0   0.00 4.16 4.65  4.01   1
203  0.12      9995.40      4.56       0.05  25.54  0.63    0   0.00 7.20 5.61  2.71   2
404  0.12      9969.15     30.50       0.34 173.55  4.66    0   0.02 6.54 5.71 18.02   3
605  0.12      9965.19     34.10       0.71 145.05  8.53    0   0.01 4.00 4.27 22.72   4
806  0.12      9994.97      4.84       0.19   4.13  1.61    0   0.00 3.00 0.86  4.54   5
1007 0.12      9982.49     16.51       1.00  93.08 12.80    0   0.01 1.29 5.65 10.27   6
```

Challenge: How to calculate the correlation coefficient for each time step?

sapply(x,f)

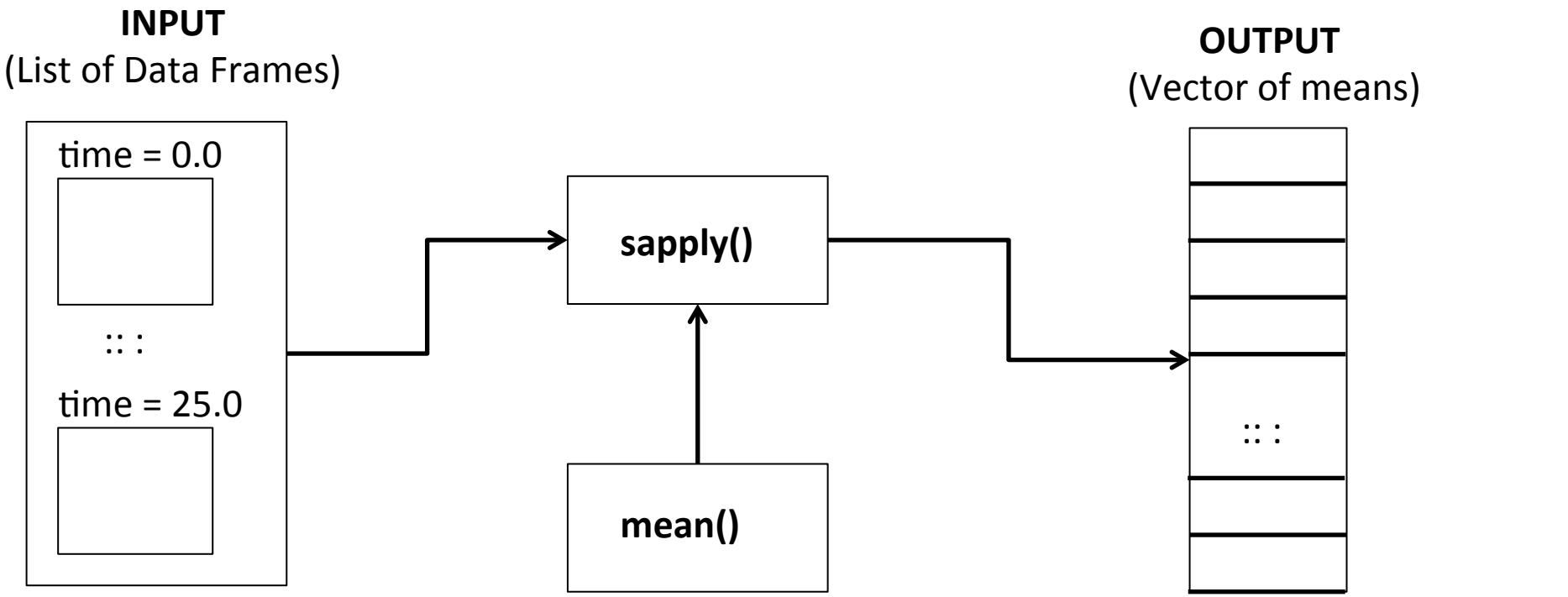
- Another use of user-defined functions in R is as parameters to the *apply* family of functions.
- The general form of the **sapply(x,f,fargs)** function is as follows:
  - **x** is the target vector or list
  - **f is the function to be called and applied to each element**
  - **fargs** are the optional set of arguments that can be applied to the function f.
  - sapply() returns a vector

Get the average at each time

using an anonymous function

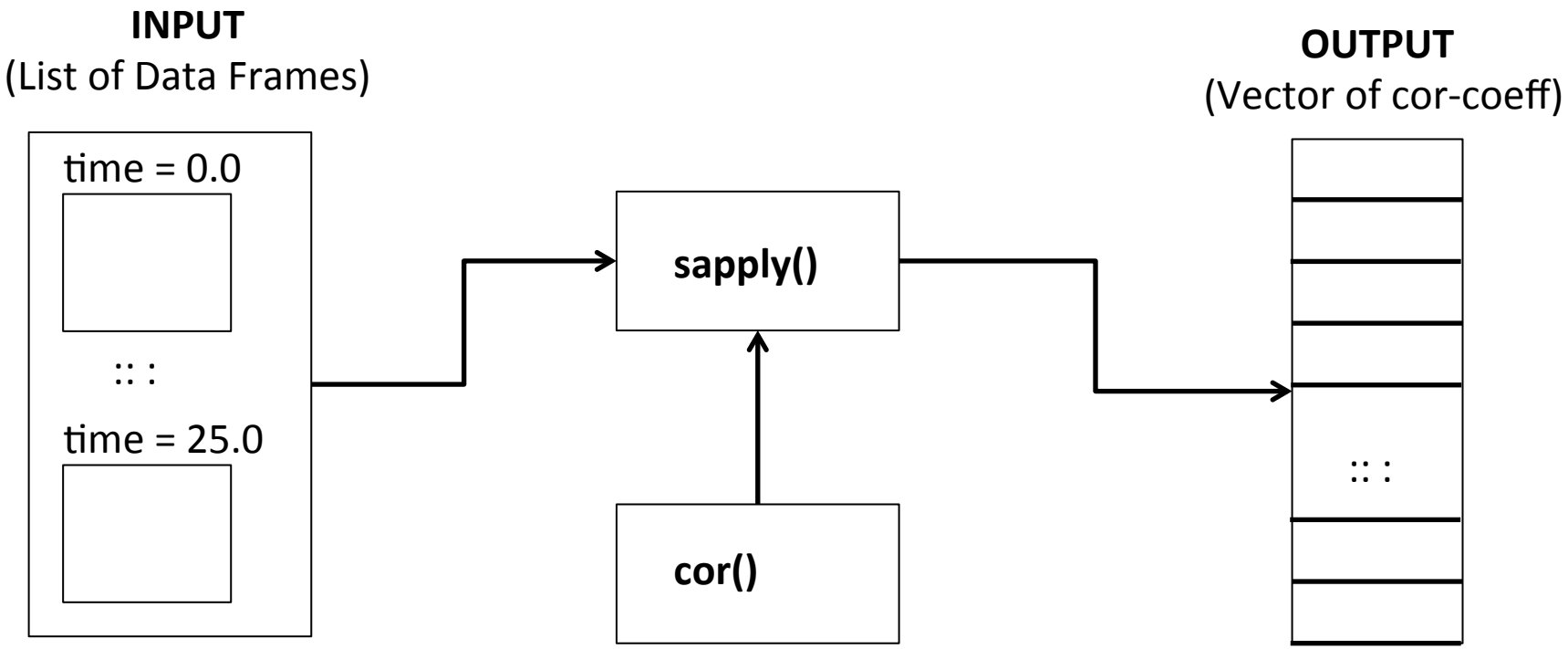
```
av.Infected<-sapply(runs,function(l){mean(l$sInfected)})
```

```
> round(av.Infected[1:10],3)
     0   0.125    0.25   0.375     0.5   0.625    0.75   0.875       1   1.125
12.997  18.196  26.327  39.230  59.956  93.535 148.129 236.543 377.490 594.582
```

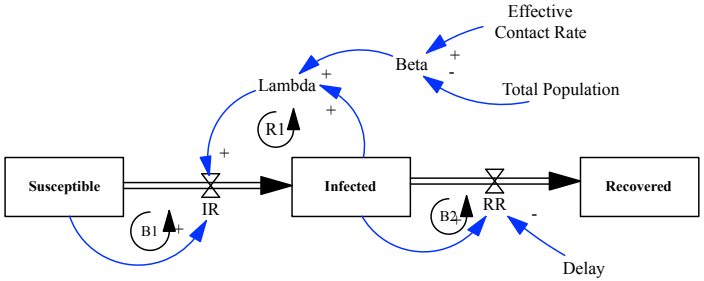


Calculating cor()

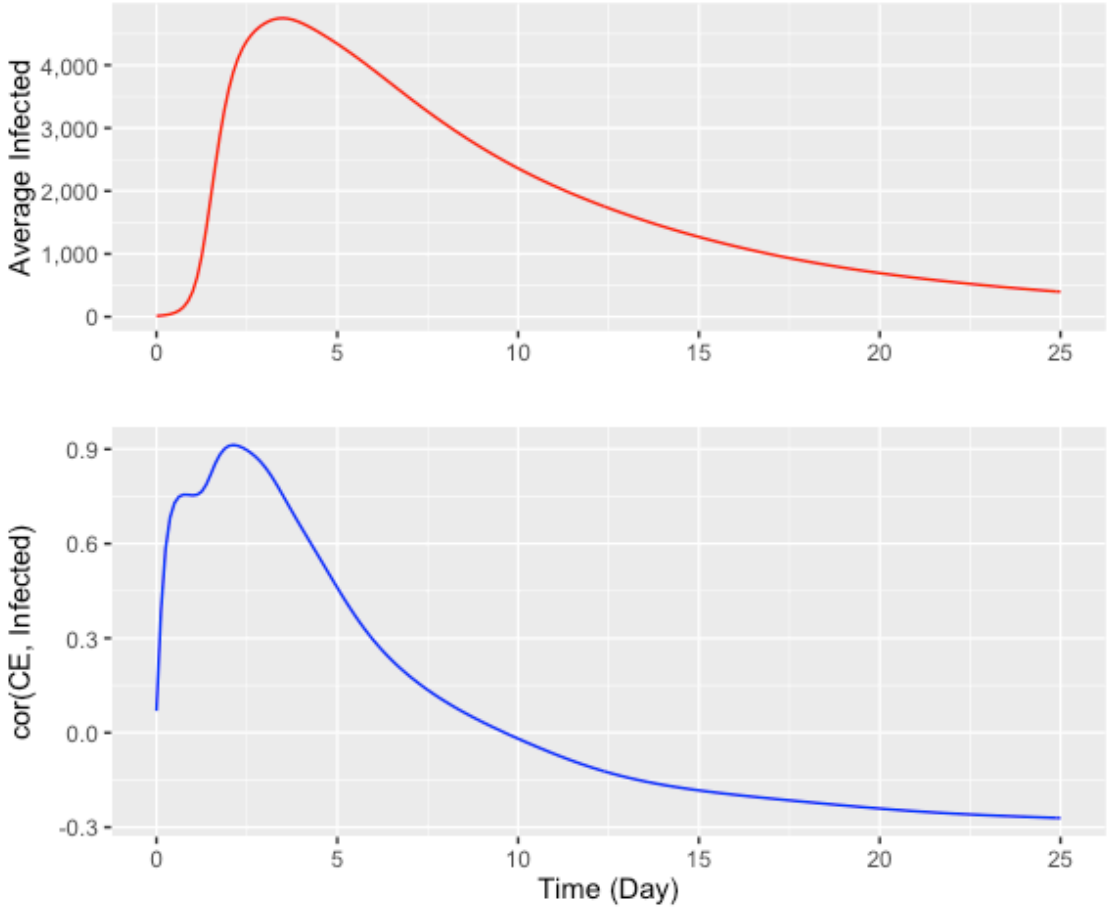
```
> cor.CE<-sapply(runs,function(l){cor(l$sInfected, l$CE)})
> round(cor.CE[1:10],3)
    0 0.125  0.25 0.375   0.5 0.625  0.75 0.875     1 1.125
0.069 0.388 0.583 0.683 0.730 0.750 0.755 0.755 0.753 0.755
```

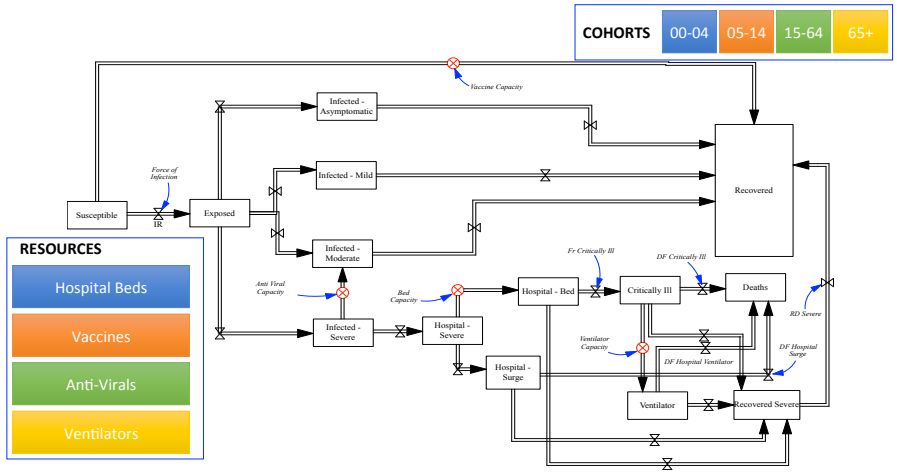


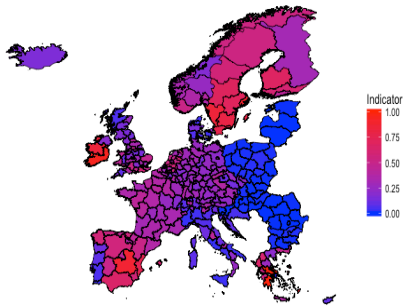
Visualising Output




```
> summary(cor.CE)
    Min.  1st Qu.   Median     Mean  3rd Qu.     Max.
-0.27090 -0.22810 -0.12640  0.06012  0.24550  0.91310
```







PANDEM

PANDEMIC RISK AND EMERGENCY MANAGEMENT

NUI Galway
OÉ Gaillimh

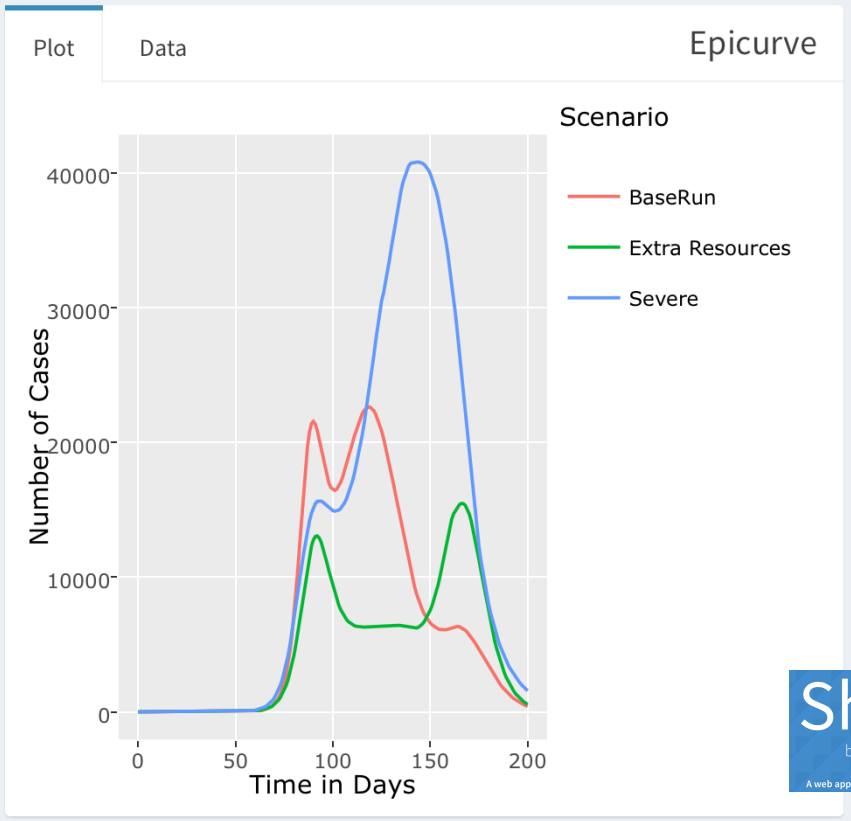
LONDON SCHOOL of HYGIENE &TROPICAL MEDICINE

World Health Organization

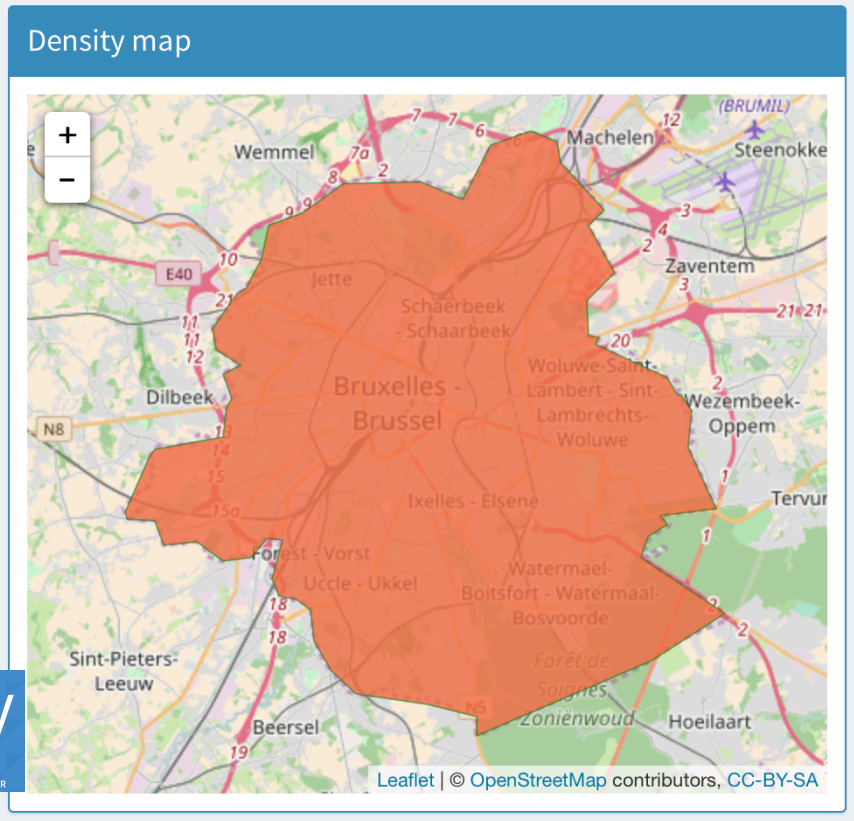
FOI

IGS

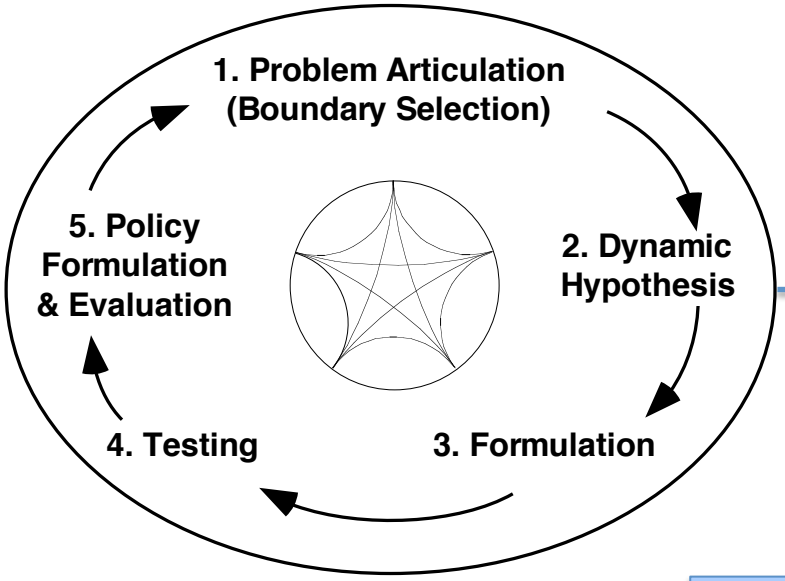
UCL
Université catholique de Louvain



Shiny
by RStudio
A web application framework for R



Summary



SD Modeling Process

R – deSolve

Data Visualisation & Exploration

R – Sensitivity & Optimisation

Sterman (2000). Business Dynamics. McGraw-Hill.

Further Reading/Resources

JimDuggan / SDMR

Unwatch 3 | Star 8 | Fork 6

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

Resources for text book "System Dynamics Modeling with R"

Edit

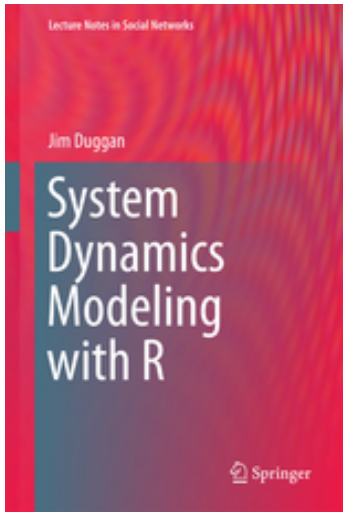
Add topics

101 commits | 1 branch | 0 releases | 1 contributor | MIT

Branch: master | New pull request | Create new file | Upload files | Find file | Clone or download

JimDuggan Update of files... Latest commit d0b4a00 2 days ago

R programming/examples	Update from lecture...	6 months ago
RShiny	Adding RShiny Tutorial (R Studio Content)	2 months ago
archive 2015	Adding lecturing archive from 2015	9 months ago
images	First draft of README summary	11 months ago
lectures/CT561	Update for energy analysis	2 months ago
models	Update for energy analysis	2 months ago
reader	Adding a pipeline delay example	4 months ago
workshops	Update of files...	2 days ago



http://link.springer.com/book/10.1007%2F978-3-319-34043-2