Gillespie Algorithm

Initialisation

Firstly, we need to install required packages.

```
## Loading required package: GillespieSSA
```

```
## Loading required package: ggplot2
```

```
## Loading required package: dplyr
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
## Loading required package: foreach
```

```
## Loading required package: reshape2
```

To do this you should use function `install.packages(package_name)`.

Gene expression model.

We will consider simple GEM defined as:

dm/dt = Sm - km * m dn/dt = Sn * m - kn * n

To simulate model using Gillespie Algorithm we will use ssa function implemented in package GillespieSSA. Let's read the ssa's documentation `?ssa`.

To simulate model we need to define:

- nu — state change matrix (stoichometric matrix)
  - rows corresponds to variables
  - columns corresponds to reactions
  - each element e_{i,j} of matrix tells what is an effect of reaction j on variable i
- a — propensity vector - prawdopodobienstwo przejscia pomiedzy stanami reakcji

```
nu <-
  matrix(
    c(1,  -1, 0, 0,
      0, 0,  1, -1),
  nrow = 2,
  byrow = TRUE)
a <-
  c("Sm",
    "km*m",
    "Sn*m",
    "kn*n")
```

Moreover we need to initiate parameters and variables state:

- x0 — initial variables state
- param — vector of parameters values
- tf — time of simulations

```
x0 <- c(m = 1, n = 0)
parms <- c(Sm = 0.05, km = 0.005, Sn = 0.05, kn = 0.001)
tf <- 5000
```

Model simulation:

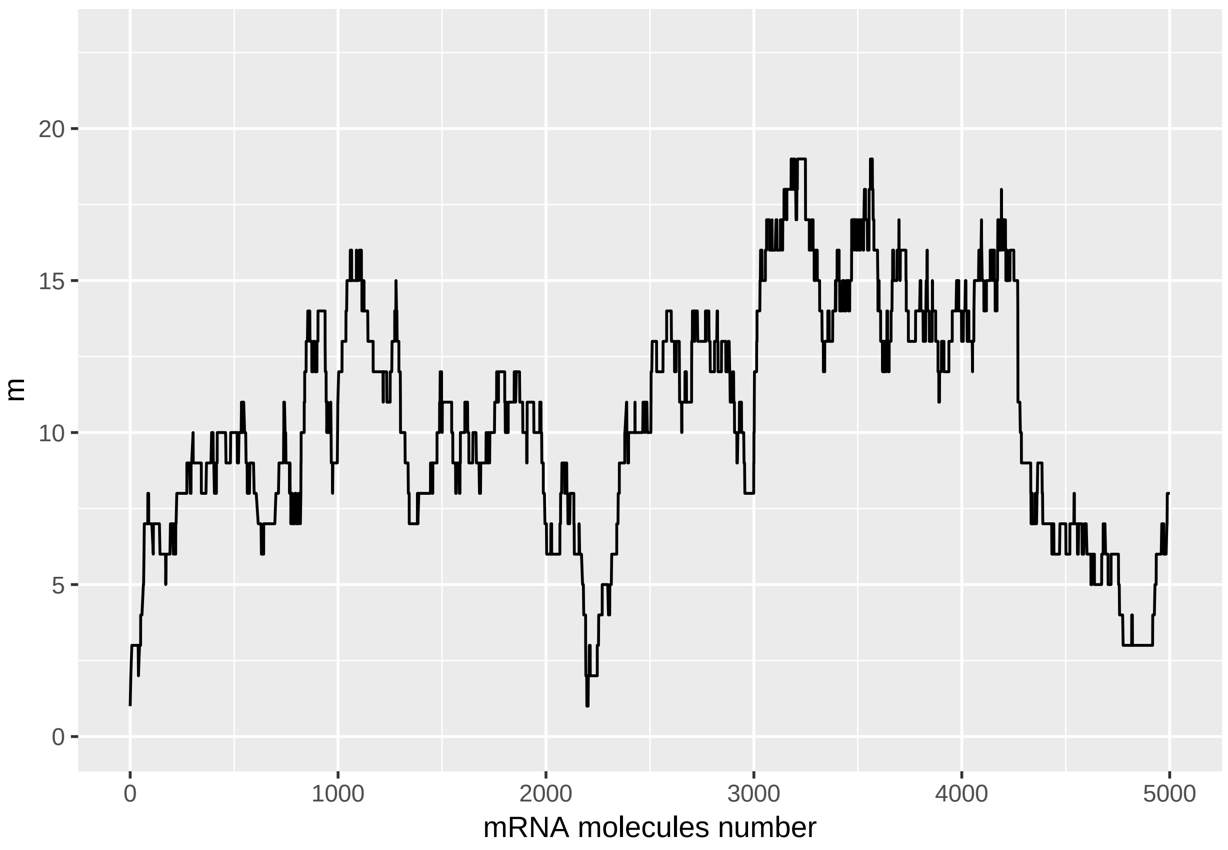
```
method <- "D"
simName <- "Gene Expression Model"
out <- ssa(x0 = x0,
           a = a,
           nu = nu,
           parms = parms,
           tf = tf,
           method = method,
           simName = simName,
           verbose = FALSE,
           consoleInterval = 1)
```

```
data <- data.frame(out$data)
colnames(data)[1] <- "t"
head(data)
```

```
##                     t m n
## timeSeries  0.000000 1 0
## X           3.113932 2 0
## X.1         7.983153 3 0
## X.2        20.434893 3 1
## X.3        22.043531 3 2
## X.4        31.781802 3 3
```

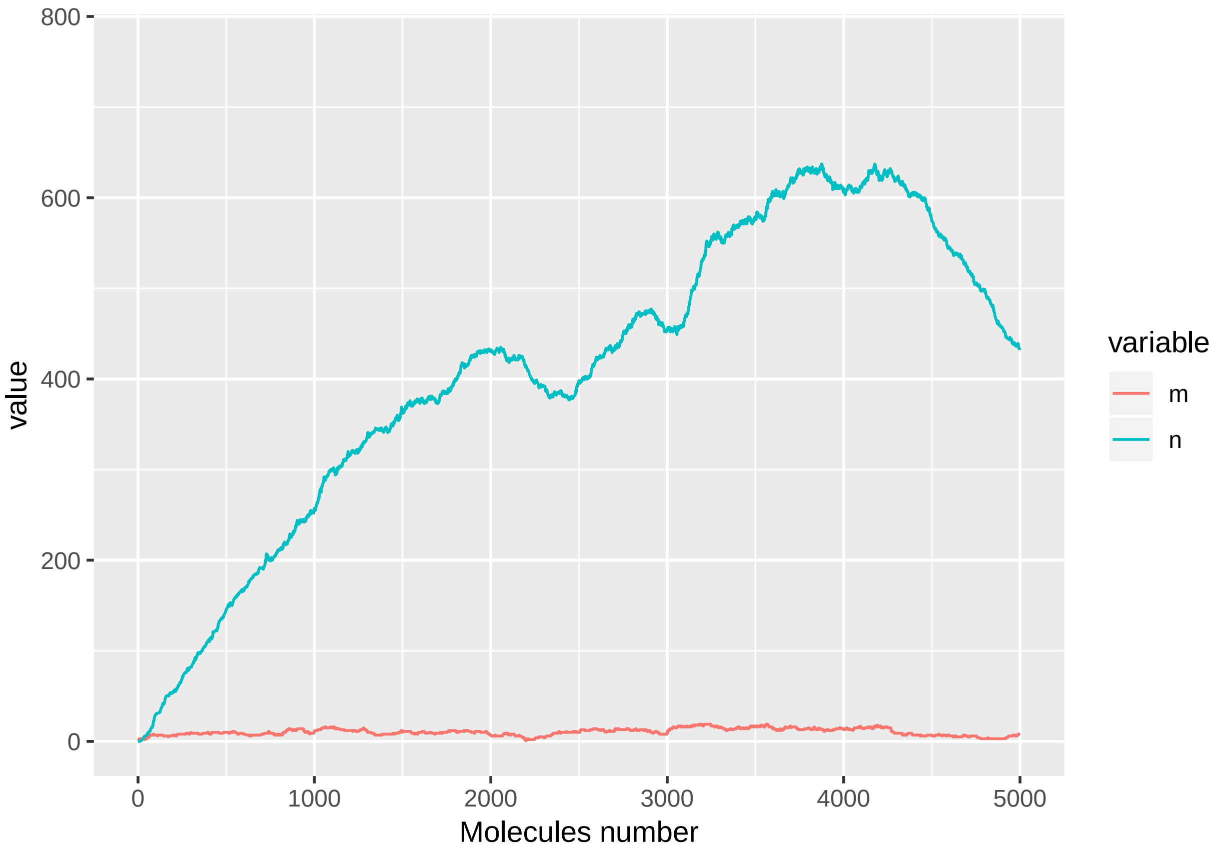
Plotting mRNA

```
g <-
  ggplot(
    data = data,
    mapping = aes(x = t, y = m)) +
  geom_line() +
  xlab("mRNA molecules number") +
  coord_cartesian(ylim = c(0, 1.2*max(data$m)))
print(g)
```



Plotting mRNA and protein in time

```r
data <- data.frame(out$data)
colnames(data)[1] <- "t"
data.long <-
  data %>%
  reshape2::melt(id = "t")
g <-
  ggplot(
    data = data.long,
    mapping = aes(x = t, y = value, group = variable, color = variable)) +
  geom_line() +
  xlab("Molecules number") +
  coord_cartesian(ylim = c(0, 1.2*max(data$m, data$n)))
print(g)
```



Task 1

Consider GEM with different initiate state values.

- Initiate in steady state
- Initiate state m = 1, n = 0
- Initiate state m = 10, n = 0

Prepare code that simulates model multiple times and plot trajectories of molecules numbers.

- Calculate and plot mean and standard deviation of molecules in time. For mRNA compare results in steady state with analytical solution of master equations.
- Calculate time of convergence to the steady state.
- Plot mRNA vs protein

Task 2

Lottka-Volter Model

- R1: A + X –> 2X
- R2: X + Y –> 2Y
- R3: Y –> *

X – rabbits Y – foxes

‘reaction’ rates: k1, k2, k3

A - paramter

- Calulcate the propensity function and stechiometric matrix
- Caluclate steady state
- Simulate model multiple times starting from different states. What is a time of convergance ?
- Prepare plot presenting population of rabbits vs foxes

Task 3

Zrób symulację następującego układu:

$A + B \rightarrow C$

$D \rightarrow A + B$

$\rightarrow E$

$E + C \rightarrow D$

$A \rightarrow *$

$B \rightarrow *$

$C \rightarrow *$

$D \rightarrow *$

$E \rightarrow *$

i znajdź taki rozkład prawdopodobieństw poszczególnych reakcji, który skutkuje dwoma scenariuszami:

układ znajduje się mniej więcej w stanie stacjonarnym układ rośnie w nieskończoność Pokaż wykresy stężeń dla wszystkich związków.

Jako stan początkowy przyjmij losowe ilości cząsteczek wszystkich związków z przedziału <2,10>.