Assignment 4

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1 Overview:

All the studied cases here will use the same assumptions which will be laid out in the next part

1.1 Steps:

- 1. Study the base case (i.e. the 1st task): infer the death rate μ by using all four curves of S, I, R, and D (after adding lognormal multiplicative noises). The structure of the pymc3 model will be changed to compare the results of different prior distributions.
- 2. Using the best combination from the first step (i.e. the best prior distributions), build a new pymc3 model without the input of the S and R curves to see if the inference of μ still works.

1.2 Assumptions:

- $\gamma = 1$, $\beta = 2.5$
- The total population (N) = 1
- Initial conditions:
 - $-i_0 = 0.01$ (fractions infected at time t=0),
 - $-s_0 = 0.99$
 - $r_0 = 0$ (fraction of recovered at time t=0)
- Time related variables:
 - $-d_0=0$,
 - f = 4.5 (time factor that defines total time window range),
 - timestep = 0.5
- Variances:
 - $-\sigma \in (0.2, 0.4)$
 - Considering that in general, the I compartment has a higher variance compared to the R and D compartments, the sigmas in this notebook will be set as: $\sigma_S = 0.25$, $\sigma_I = 0.38$, $\sigma_R = 0.22$, $\sigma_D = 0.20$
- *R*₀ (R nought):
 - Since R_0 (R nought) = $\frac{\beta}{\gamma + \mu}$, $\gamma = 1$, $\beta = 2.5$, R_0 (R nought) = $\frac{2.5}{1 + \mu}$
 - Therefore, $\mu = \frac{2.5}{R_0}$ -1
- Value ranges of R_0 (R nought) and μ :
 - Given the relationship between the death rate μ and R_0 (R nought), and it is obvious that $\mu \in [0, 1]$, the range for R_0 (R nought) can also be inferred.
 - − By combining these two expressions, it turns out that R_0 (R nought) ∈ [1.25, 2.5] This value range will be applied later in the MCMC model, where a bounded prior distribution is assumed for R_0 (R nought)

1.3 Note:

- While the goal of performing MCMC is to infer the death rate μ , the actual process shown here is for inferring the R_0 (R nought), and therefore posterior distributions of R_0 (R nought) will be presented instead.
- Considering the assumption of this notebok, this is essentially the same as inferring the death rate μ . As mentioned before, as γ is fixed to be 1, R_0 (R nought) = $\frac{2.5}{1+\mu}$. Therefore, once R_0 (R nought) can be inferred, the death rate μ can also be determined.

```
[1]: # Import Python packages
   import pandas as pd
   import numpy as np
   np.random.seed(42)

import matplotlib.pyplot as plt
%precision 4
%matplotlib inline

import pymc3 as pm
from pymc3.ode import DifferentialEquation
from scipy.integrate import odeint

import warnings
from warnings import simplefilter
warnings.filterwarnings("ignore")
simplefilter(action='ignore', category=FutureWarning)
```

```
[2]: # Import two python files made for this assignment (should be # in the same folder), more descriptions can be found in # these two .py files from SIRD import SIRD, IRD, SID from MCMC import MCMC, MCMC_model
```

```
[3]: # Define initial conditions of SIRD model
i0, r0, d0 = 0.01, 0.00, 0.00
s0 = 1-i0-r0-d0

# Time-related definitions
f, timestep_data = 4.5, 0.5
times = np.arange(0,5*f,timestep_data)

# Assumptions of infection rate, recovery rate, and sigmas of
# noises for the SIRD curves
beta, gamma = 2.5, 1
sigmas = [0.25, 0.38, 0.22, 0.20]

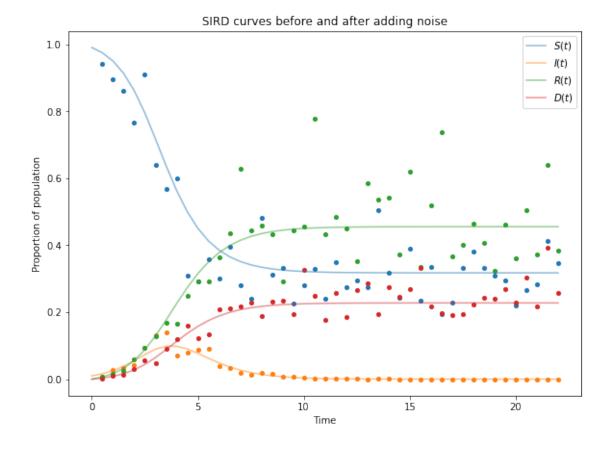
# Ground truth (fixed gamma=1 and beta=2.5, then R0=2.5/(1+mu),
```

```
# time scale to t/gamma)
mu = 0.5
R0 = 2.5/(1+mu)
```

2 Part I. Base case

Goal: infer the death rate μ , given noisy S(t), I(t), R(t), D(t) input curves.

```
[4]: y = \text{odeint}(SIRD, t=\text{times}, y0=[s0, i0, r0, d0],
                args=([2.5/(1+mu)],), rtol=1e-8)
     yobs = np.zeros([len(times)-1,np.shape(y)[1]])
     # To avoid situations where the value of S/I/R/D, after adding noise,
     # become larger than 1 (which is not realistic, as S/I/R/D represent
     # the proportion of the population), a multiplicative noise is added
     # to each data point of the four curves in turn:
     for i in range(np.shape(y)[1]):
         for j in range(len(times)-1):
             while True:
                 yobs[j,i] = np.random.lognormal(mean=np.log(y[j+1,i]),
                                                  sigma=sigmas[i])
                 if yobs[j,i] <= 1: # check if the noise added data point is realistic
                     break
     fig1, ax1 = plt.subplots(1,1,figsize=(8,6),constrained_layout=True)
     ax1.plot(times[1::], yobs, marker='o', linestyle='none', markersize=4)
     ax1.plot(times, y[:,0], color = 'CO', alpha=0.5, label=f'$S(t)$')
     ax1.plot(times, y[:,1], color = 'C1', alpha=0.5, label=f'$I(t)$')
     ax1.plot(times, y[:,2], color='C2', alpha=0.5, label=f'$R(t)$')
     ax1.plot(times, y[:,3], color = 'C3', alpha=0.5, label=f'$D(t)$')
     ax1.legend()
     ax1.set_title('SIRD curves before and after adding noise')
     ax1.set_xlabel('Time')
     ax1.set_ylabel('Proportion of population')
     plt.show()
```



2.1 Note regarding the imported MCMC.py file:

The MCMC models in this notebook are built using functions stored in the MCMC.py, which has two ways of building the model:

• By calling the function MCMC, which is an interactive function that allows users to customize the model parameters to some extent by inputting different instructions. The available options for customization will be shown in the demonstration example shown in the next part (i.e. which number represents which prior distributions for sigmas and R_0 (R nought). Therefore, the sample size in the Demo and the tuning number is very small as it's not part of the real analysis section.

For more descriptions, please refer to the MCMC.py file.

• By calling the function MCMC_model (which will be used after the Demo for the MCMC function). This arguments for MCMC_model are essentially the same as MCMC (the number labels for the distribution choices are the same).

For more descriptions, please refer to the MCMC.py file.

2.2 Case (0): Demo for function MCMC (which uses interactive input)

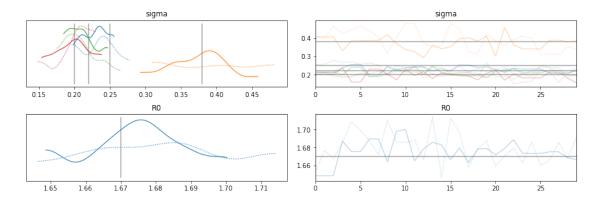
```
[6]: initial = [s0, i0, r0, d0] # vector of initial conditions
     summary_0 = MCMC(sird_model=sird_model, # used for constructing
                                            # the curves in MCMC modeling
                     initial=initial, yobs=yobs,
                     sample_size=30, tune=10,
                     sigmas=sigmas, RO=RO) # true sigma and R nought values
                                           # are provided for the final graph
                                           # output so that the accuracy of
                                           # the model can be evaluated
    Please input the label (integer) of the prior distribution of sigmas.
    (1--Half Cauchy; 2--Half Normal; 3--Bounded Half Cauchy; 4--Bounded Half Normal)
    1
    Please input the parameter of the prior distribution of sigmas.
    (For Half Cauchy distributions the parameter is Beta, and for Half Normal
    distributions the parameter is sigma.)
    1
    Please input the label (integer) of the prior distribution of RO.
    (1--Bounded Normal; 2--Bounded Logormal)
    Please input the parameters of the prior distribution of RO, i.e. mean and sigma
    of the distribution: (needs to be in list formate.g., mean=2 and sigma=3
    expressed as [2,3])
    [2,2.5]
                            MCMC modeling starts from here
                            _____
    <IPython.core.display.HTML object>
    Only 30 samples in chain.
    Sequential sampling (2 chains in 1 job)
    NUTS: [RO, sigma]
```

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

Sampling 2 chains for 10 tune and 30 draw iterations (20 + 60 draws total) took 22 seconds.

Assuming the distributions of sigmas are Half Cauchy, and distribution of RO is Bounded Normal.



2.2.1 Analysis of output graphs in (0):

- As mentioned before, this section is intended only for demonstration, therefore a very small sample size (30) and tuning number (10) was used.
- The two graphs on the left above represent the posterior distributions of the sigmas and R_0 (R nought) output by the MCMC model. The vertical lines in these two plots represent the true values of the parameters. It can be seen that the distributions output are all roughly around the true values. Therefore, even when given very few samples, the model was already able to approximately capture the parameters' true values.
- The two graphs on the right shows the changes of the parameters' values for each sample, and the horizontal lines in them represent the true values. A similar observation can be made for these two graphs: the model was able to approximately capture the true values of these parameters with a very small number of sample size.

2.3 Start analysis by using function MCMC_model

2.3.1 Note:

Although there are many more combinations, only three cases are shown in this notebook. This is because after trying out other combinations, it appears that the differences between them are very small, which will be shown later.

```
[7]: import time start_time = time.time()
```

2.4 Case (1): Initial combination

In this case, Half Cauchy distribution is used for prior of sigma, and Bounded Normal distribution is used for prior of R_0 (R nought)

<IPython.core.display.HTML object>

Only 400 samples in chain. Sequential sampling (2 chains in 1 job)

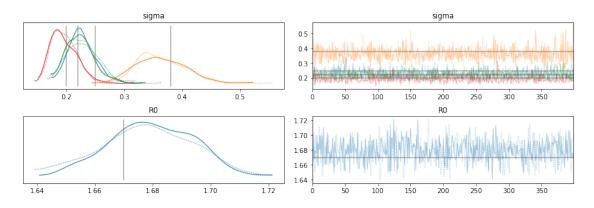
NUTS: [RO, sigma]

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

Sampling 2 chains for 1_000 tune and 400 draw iterations ($2_000 + 800$ draws total) took 715 seconds.

Assuming the distributions of sigmas are Half Cauchy, and distribution of RO is Bounded Normal.



Analysis of output graphs in (1):

• The two graphs on the left above represent the posterior distributions of the sigmas and R_0 (R nought) output by the MCMC model. The vertical lines in these two plots represent the

true values of the parameters. It can be seen that the distributions output are all roughly around the true values. Moreover, compared with the case in (0) which has small sample size, these posteriors are smoother and have smaller variance between the two chains (represented by the solid and the dotted lines).

• The two graphs on the right shows the changes of the parameters' values for each sample, and the horizontal lines in them represent the true values. A similar observation can be made for these two graphs: the model was able to better capture the true values of these parameters with a larger sample size.

2.5 Case (2): First variation - change the prior distribution for sigmas

Prior distributions for sigmas are changed from Half Cauchy to Half Normal, while and their parameter values are changed from beta=1 to beta=1.5

<IPython.core.display.HTML object>

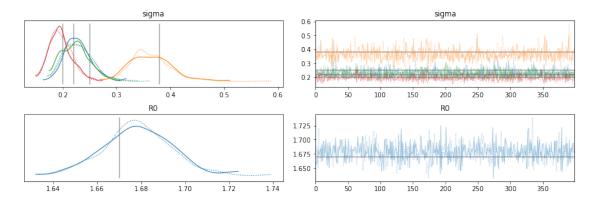
```
Only 400 samples in chain.
Sequential sampling (2 chains in 1 job)
NUTS: [RO, sigma]
```

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

Sampling 2 chains for 1_{-000} tune and 400 draw iterations (2_{-000} + 800 draws total) took 702 seconds.

Assuming the distributions of sigmas are Half Normal, and distribution of RO is Bounded Normal.



2.5.1 Analysis of output graphs in (2):

- The two graphs on the left above represent the posterior distributions of the sigmas and R_0 (R nought) output by the MCMC model. The vertical lines in these two plots represent the true values of the parameters. By changing the prior distributions for the sigmas, the effect on the model's output is very little—the shapes of the posteriors as well as the relationship between the posteriors and the true values are barely changed.
- The two graphs on the right shows the changes of the parameters' values for each sample, and the horizontal lines in them represent the true values. A similar observation can be made for these two graphs: the model has shown very few changes compared to the graphs in (1) when the priors for sigmas are changed.

2.6 Case (3): Second variation - change the prior distribution for R_0

The prior distribution for R_0 is changed from Bounded Normal to Bounded Lognormal, and its parameter values are changed from [mean=2, variance=2.5] to [mean=1.8, variance=2]

<IPython.core.display.HTML object>

```
Only 400 samples in chain.

Sequential sampling (2 chains in 1 job)

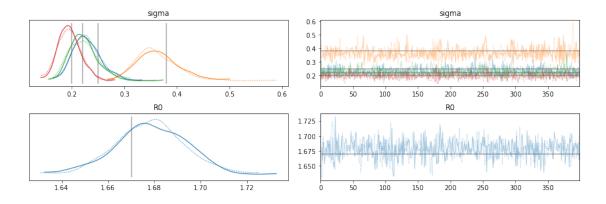
NUTS: [R0, sigma]

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

Sampling 2 chains for 1_000 tune and 400 draw iterations (2_000 + 800 draws total) took 711 seconds.
```

Assuming the distributions of sigmas are Half Cauchy, and distribution of RO is Bounded Lognormal.



2.6.1 Analysis of output graphs in (3):

- The two graphs on the left above represent the posterior distributions of the sigmas and R_0 (R nought) output by the MCMC model. The vertical lines in these two plots represent the true values of the parameters. By changing the prior distributions for R_0 (R nought), the effect on the model's output is very little—the shapes of the posteriors as well as the relationship between the posteriors and the true values are barely changed.
- The two graphs on the right shows the changes of the parameters' values for each sample, and the horizontal lines in them represent the true values. A similar observation can be made for these two graphs: the model has shown very few changes compared to the graphs in (1) when the prior for R_0 (R nought) is changed.

```
[11]: end = time.time()
print("Time spent: ", end-start_time)
```

Time spent: 2626.4950189590454

2.7 Initial conclusion based on analysis of the traceplots above:

By changing the priors for sigmas or changing the prior for R_0 (R nought), it appears that the results of the MCMC model have shown very small changes. Therefore, the next section will analyze the differences between these cases from a numerical perspective.

2.7.1 Relate back to the summary tables for the three cases:

Results of the three runs are summarized in summary_1 (initial case), summary_2 (only changing sigmas priors), and summary_3 (only changing R_0 prior)

As the traceplots showed previously, changing the distributions didn't lead to much improvement. Therefore, the changes in these summary tables are expected to be very limited. Therefore, for demonstration purpose, only the values of the mean column in these tables are used as the other columns are not so important here.

To evaluate these three cases, these mean values can be compared with their corresponding true values to see how close they are to each other.

```
[12]: # Construct a dataframe to store all the mean columns
      mean_df = pd.concat([summary_1['mean'],
                           summary_2['mean'],
                           summary_3['mean']],
                          axis=1)
      # Rename columns
      mean_df.columns=['Initial_case', '1st_variation', '2nd_variation']
      # Insert a column for the corresponding true values
      true_value = sigmas
      true_value.append(R0)
      mean_df['True_value'] = true_value
      # Calculate the (absolute) differences between the mean values and
      # their corresponding true values
      for i in range(3):
          mean_df.iloc[:,i] = abs(mean_df.iloc[:,i]-mean_df['True_value'])
      # Drop the true value column and visualize the differences of the
      # three cases
      mean_df = mean_df.drop('True_value', axis=1)
      mean_df.style.background_gradient(cmap='PuBu', axis=1)
```

[12]:

sigma[0]	0.022000	0.022000	0.021000
sigma[1]	0.016000	0.015000	0.017000
sigma[2]	0.004000	0.006000	0.003000
sigma[3]	0.004000	0.004000	0.004000
R0	0.012333	0.011333	0.011333

Initial case 1st variation 2nd variation

2.7.2 Analysis of the summary tables:

After subtracting the true values from the mean values output by the three models and taking their absolute values (as the "absolute deviation" is the focus here), the cells are color coded as shown above based on the comparisons across each row (i.e. in the first row, the values 0.022, 0.022, and 0.021 are compared and since the first two are the highest, they are given a dark color). Again, the differences between the three cases are very small, as mentioned above. Even so, the third column, which has the fewest dark colored cells, have shown a (slight) advantage over the other cases.

3 Part II. Study the effect of removing the S and R curves

In this part, the focus is on the curves fed into the MCMC models themselves instead of the model accuracy. Therefore, the same set of parameters of the model will be used. Since it has been shown previously that the different sets of parameters don't seem to make much difference, any of the three cases can be used. Here, the combination that we choose are:

- 1. Prior for sigmas: Half Cauchy with $\beta = 1$
- 2. Prior for R_0 (R nought): Bounded Lognormal with mean=1.8 and sigma=2

To study the effect of removing the S and R curves, two cases are presented here:

1. Only removing the S curve. In this case, it is essentially the same as removing both S and R curves, the reason is shown as follows: as stated in the assumptions, β and γ have fixed values. Therefore, the value of μ can be inferred if the value of R_0 (R nought) is provided. As

$$\frac{dR}{dt} = \frac{\gamma I}{N}$$

and

$$\frac{dD}{dt} = \frac{\mu I}{N}$$

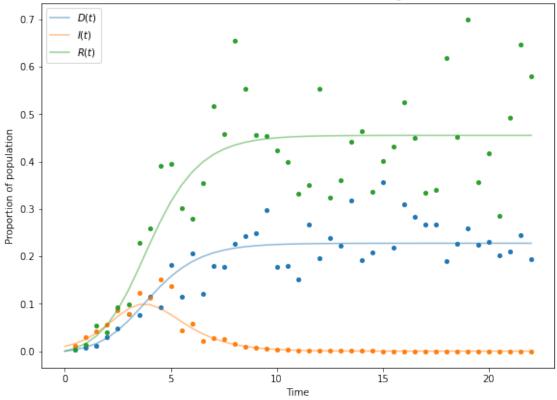
—then if the I curve can be calculated, then given that μ can be inferred, even when R curve is not provided, it can still be calculated.

2. Only removing the R curve.

3.1 Case (1): Removing S curve (keeping only I, R, and D curves)

```
# Plot the deterministic curves, and those with multiplicative noise
fig2, ax2 = plt.subplots(1,1,figsize=(8,6),constrained_layout=True)
ax2.plot(times[1::], yobs, marker='o', linestyle='none', markersize=4)
ax2.plot(times, y[:,0], color ='CO', alpha=0.5, label=f'$D(t)$')
ax2.plot(times, y[:,1], color ='C1', alpha=0.5, label=f'$I(t)$')
ax2.plot(times, y[:,2], color ='C2', alpha=0.5, label=f'$R(t)$')
ax2.legend()
ax2.set_title('I, D, and R curves before and after adding noise')
ax2.set_xlabel('Time')
ax2.set_ylabel('Proportion of population')
plt.show()
```





```
n_states=3, # I, R, and D are states
n_theta=1, # R0 is the only parameter
t0=0) # start from zero
```

<IPython.core.display.HTML object>

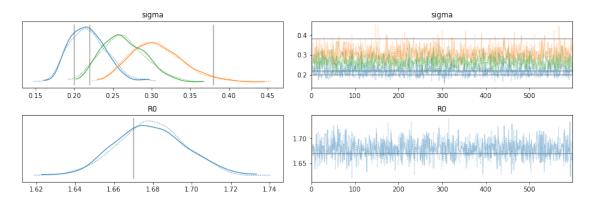
Sequential sampling (2 chains in 1 job) NUTS: [RO, sigma]

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

Sampling 2 chains for 1_{-000} tune and 600 draw iterations ($2_{-000} + 1_{-200}$ draws total) took 642 seconds.

Assuming the distributions of sigmas are Half Cauchy, and distribution of RO is Bounded Lognormal.



3.1.1 Analysis of output graphs in (1):

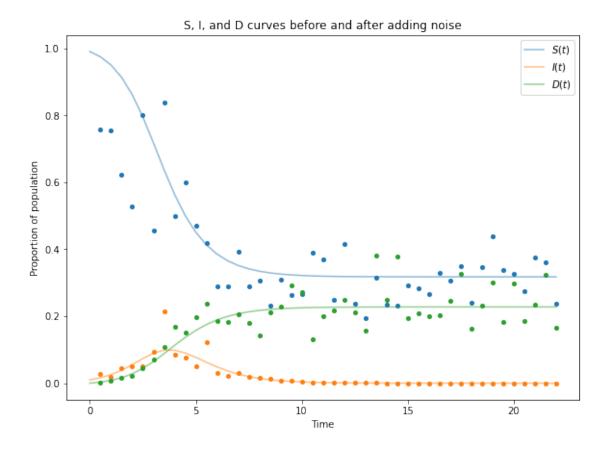
• The two graphs on the left above represent the posterior distributions of the sigmas and R_0 (R nought) output by the MCMC model. The vertical lines in these two plots represent the true values of the parameters. When only I, R, and D curves are provided, it appears that the posterior distributions of sigmas have performed more poorly compared to the ones in Part I where all four curves are provided. In comparison, the posterior distribution of R_0 (R nought) seems to have barely changed and can still approximately capture the true value.

• The two graphs on the right shows the changes of the parameters' values for each sample, and the horizontal lines in them represent the true values. A similar observation can be made for these two graphs: the model's performance is worse in the case of the sigma values, while in the case of R_0 (R nought), limited changes can be observed.

3.2 Case (2): Removing R curve (keeping only S, I, and D curves)

```
[17]: del y, yobs, initial
initial = [s0, i0, d0]
sigmas_3 = [0.25, 0.38, 0.20]
```

```
[18]: # Create S, I, and D curves
      y = odeint(SID, t=times, y0=[s0, i0, d0],
                 args=([2.5/(1+mu)],), rtol=1e-8)
      yobs = np.zeros([len(times)-1,np.shape(y)[1]])
      # To avoid cases where noise-added data points have values
      # above 1, same process is performed as above in Part I
      for i in range(np.shape(y)[1]):
          for j in range(len(times)-1):
              while True:
                  yobs[j,i] = np.random.lognormal(mean=np.log(y[j+1,i]),
                                                  sigma=sigmas_3[i])
                  if yobs[j,i] <= 1: # check if the noise added data point is realistic
                      break
      # Plot the deterministic curves, and those with multiplicative noise
      fig3, ax3 = plt.subplots(1,1,figsize=(8,6),constrained_layout=True)
      ax3.plot(times[1::], yobs, marker='o', linestyle='none', markersize=4)
      ax3.plot(times, y[:,0], color ='CO', alpha=0.5, label=f'S(t)')
      ax3.plot(times, y[:,1], color = 'C1', alpha=0.5, label=f'$I(t)$')
      ax3.plot(times, y[:,2], color ='C2', alpha=0.5, label=f'$D(t)$')
      ax3.legend()
      ax3.set_title('S, I, and D curves before and after adding noise')
      ax3.set_xlabel('Time')
      ax3.set_ylabel('Proportion of population')
      plt.show()
```



<IPython.core.display.HTML object>

Sequential sampling (2 chains in 1 job)

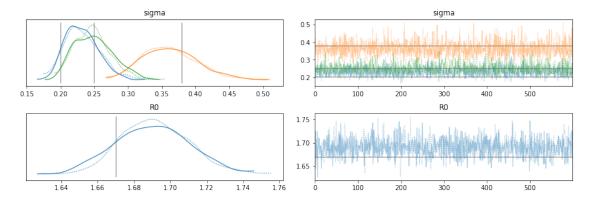
NUTS: [RO, sigma]

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

Sampling 2 chains for 1_000 tune and 600 draw iterations (2_000 + 1_200 draws total) took 656 seconds.

Assuming the distributions of sigmas are Half Cauchy, and distribution of RO is Bounded Lognormal.



3.2.1 Analysis of output graphs in (2):

- The two graphs on the left above represent the posterior distributions of the sigmas and R_0 (R nought) output by the MCMC model. The vertical lines in these two plots represent the true values of the parameters. When only S, I, and D curves are provided, it appears that the posterior distirbutions of the sigmas are not very different from the ones in Part I where all four curves are provided. In comparison, the posterior distribution of R_0 (R nought) has shown more deviation from the true value.
- The two graphs on the right shows the changes of the parameters' values for each sample, and the horizontal lines in them represent the true values. A similar observation can be made for these two graphs: the model's performance is worse in the case of the R_0 (R nought) values, while in the case of the sigmas, limited changes can be observed.

4 Conclusion

• As shown in Part I, where all four curves of S, I, R, and D are provided, the changes in the prior distributions of eigher sigmas or R_0 (R nought) have very limited effects on the MCMC model's performance. Therefore, if one intends to optimize the code here, one should approach from a perspective of improving the computing speed instead of the perspective of improving the model's output. As the computing times in this notebook are relatively acceptable, this optimization is therefore not considered at the moment. For future reference,

one might try other available pakcages designed for MCMC that might allow for more efficient parallelized computing.

- As shown in Part II, where only 3 out of the previous 4 curves are provided, the MCMC model can still output a fairly accurate estimate of the R_0 (R nought). Since the values of R_0 (R nought) and death rate μ can be computed from each other (using R_0 (R nought) = $\frac{2.5}{1+\mu}$), it can be concluded that with the removal of the S and/or R curves, the model can still infer the value of μ (although the accuracy might suffer as a result as shown in Part II's analysis).
 - Meanwhile, it is interesting to see that for the two cases in Part II, different observations are made regarding the models' accuracy–compared with Part I, when the S curve is removed, the accuracy of sigmas predictions have dropped while the accuracy of R_0 (R nought) prediction shows very small changes, and when the R curve is removed, the effects are the opposite (the accuracy of sigmas predictions barely changed while the accuracy of R_0 (R nought) prediction decreased). At the moment we cannot come up with a reasonable explanation for this phenomenon, which can be one of the topics for future work.
- Other comments for future work: for simplicity, the noise adding process for the curves are performed separately without constraints. However, this is not realistic: even after adding noises, the four curves should add up to 1 at any time point.