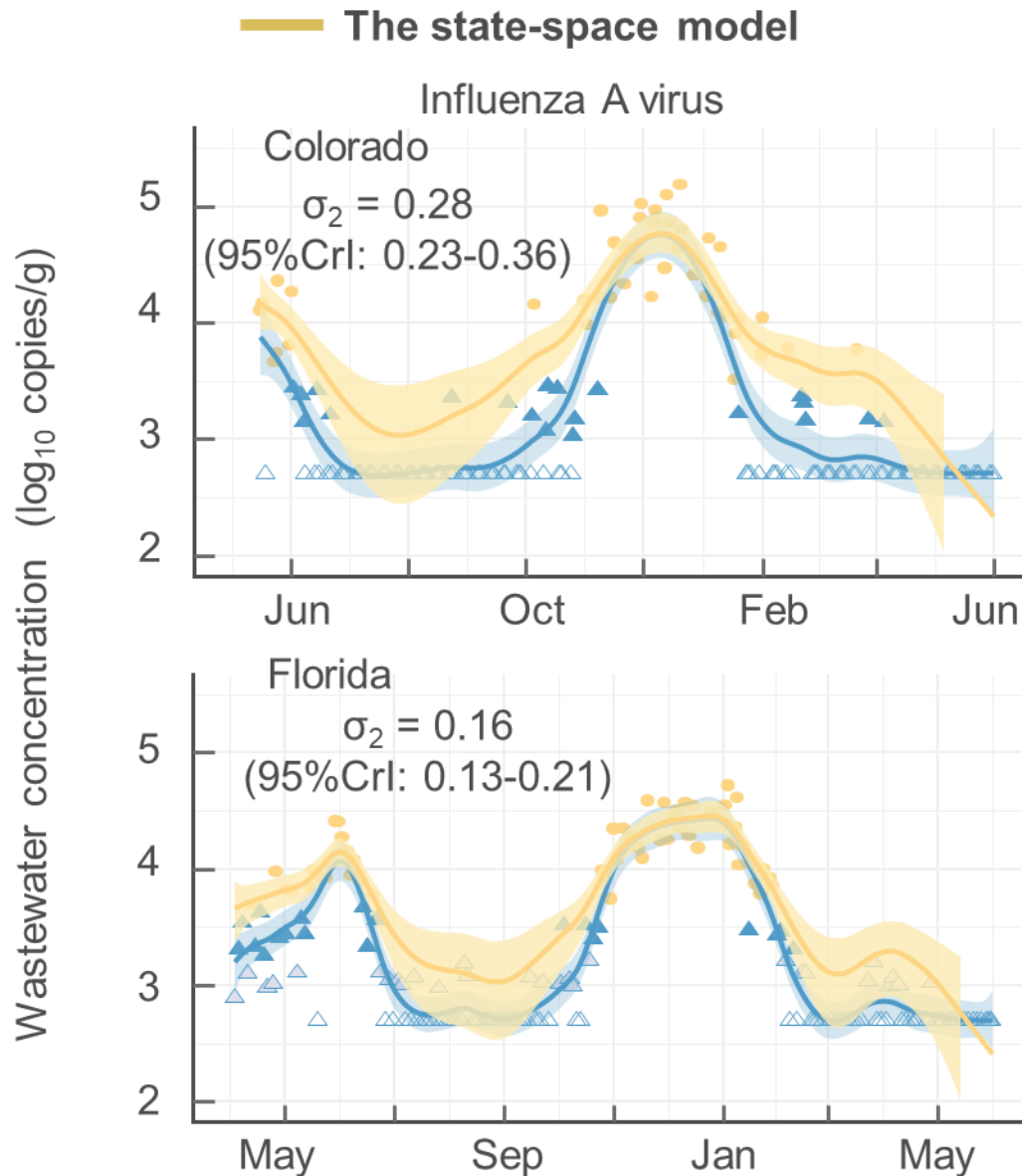


Brief guide for using the state-space model



Content

Name of used R and stan files

(state_space_model_with_logistic.R)

(state_space_model_with_logistic.stan)

- Install and download (slide: 2 ~ 3)
- Import wastewater-based data (slide: 4 ~ 9)
- Set prior distribution (slide 10)
- Implement analysis (slide 11 ~ 13)

Name of used R and stan files

(state_space_model_with_logistic_highspeed.R)

(state_space_model_with_logistic_highspeed.stan)

- High speed analysis

Contact: hirokiando@arizona.edu

- Install “R” and “Rstudio”

<https://rstudio-education.github.io/hopr/starting.html>

- Download R file, csv file, and stan file from the github.

202410_WBE_censored_data (Private)

Unwatch 1 Fork 0 Star 0

main 2 Branches 0 Tags

Go to file Add file Code

Hiroki-Ando1998 Update state_space_model_with_logistic_highspeed.R 9d79eab · 2 months ago 57 Commits

File	Update	Time
Analysis of real-world data	Update 20240823_Figure_4_RSV_2_substitution.R	4 months ago
Figure	Add files via upload	4 months ago
Raw data on wastewater concentration of IAV ...	Delete Raw data on wastewater concentration of IAV and RS...	4 months ago
Simulation	Update 20240809_WBE_ND_simulation_1.R	5 months ago
Protocol for the state_space_model.pdf	Add files via upload	4 months ago
state_space_model_with_logistic.R	Update state_space_model_with_logistic.R	3 months ago
state_space_model_with_logistic.stan	Add files via upload	4 months ago
state_space_model_with_logistic_highspeed.R	Update state_space_model_with_logistic_highspeed.R	2 months ago
state_space_model_with_logistic_highspeed.stan	Update ... rename state_space_model_with_logistic_highsp...	2 months ago
template_example_file.xlsx	Add files via upload	4 months ago
template_file.csv	Add files via upload	4 months ago

About
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Languages
R 92.1% Stan 7.9%

Files

main + Q

Go to file

Analysis of real-world data

Figure

Raw data on wastewater concentr...

Simulation

Protocol for the state_space_mod...

state_space_model_with_logistic.R

state_space_model_with_logistic.s...

state_space_model_with_logistic_...

state_space_model_with_logistic_...

template_example_file.xlsx

template_file.csv

202410_WBE_censored_data state_space_model_with_logistic.R

Hiroki-Ando1998 Update state_space_model_with_logistic.R d1c517f · 3 months ago History

Code Blame 178 lines (136 loc) · 5.92 KB Code 55% faster with GitHub Copilot

Raw Download

```

1
2 getwd() #check where you should upload csv file analyzed
3
4 install.packages("dplyr")
5 install.packages("tidyr")
6 install.packages("plyr")
7 install.packages("ggplot2")
8 install.packages("rstan")
9 install.packages("stats")
10 install.packages("bayesplot")
11
12 library(dplyr)
13 library(tidyr)
14 library(plyr)
15 library(ggplot2)
16 library(rstan)
17 library(stats)

```

- Open the CSV file downloaded in your laptop
- Input wastewater-based data in the template CSV file

A	B	C	D	E
date	number_of_tested_sa	number_of_positive_samples	concentration	
2022/1/1				
2022/1/2				
2022/1/3	2	2	30955.34439	
2022/1/4	3	3	24419.80553	
2022/1/5				
2022/1/6	NA	NA	NA	
2022/1/7	NA	NA	NA	
2022/1/8	2	1	1334.963692	
2022/1/9	5	3	1842.572202	
2022/1/10	5	3	2632.292098	
2022/1/11	5	3	3171.828039	
2022/1/12	4	3	2149.002467	
2022/1/13	5	2	4058.253557	
2022/1/14	4	1	13460.97495	

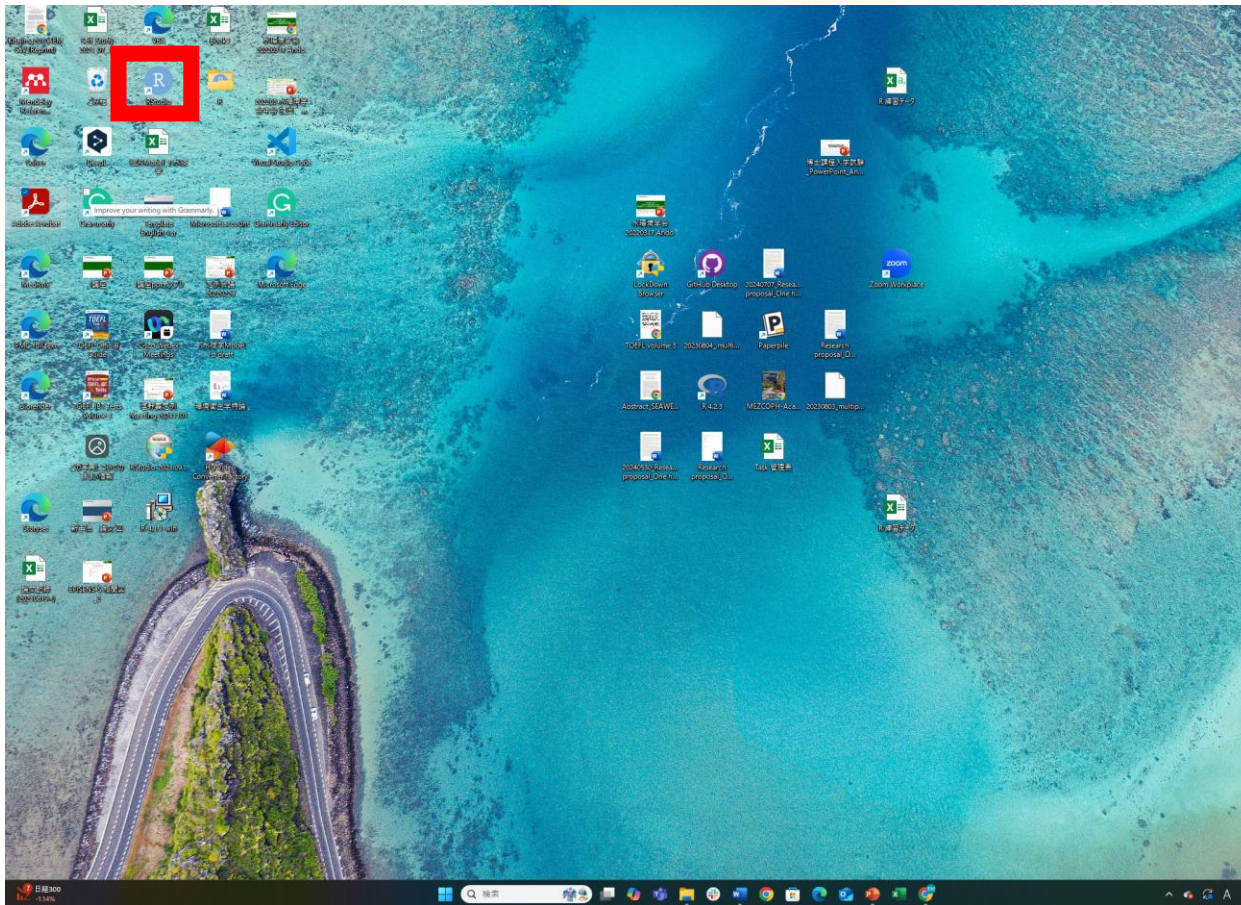
Data in non sampling day should be blank or “NA”.

↑
Integer

↑
Integer

↑
Copies/L

- Open “Rstudio” in your desktop



- Check where you have to upload CSV file, R and Stan file.

Console Terminal Background Jobs

R 4.2.3 - C:/2023_R/

```
R version 4.2.3 (2023-03-15 ucrt) -- "Shortstop Beagle"
Copyright (C) 2023 The R Foundation for Statistical Computing
Platform: x86_64-w64-mingw32/x64 (64-bit)

R は、自由なソフトウェアであり、「完全に無保証」です。
一定の条件にばえば、自由にこれを再配布することができます。
配布条件の詳細に関しては、'license()' あるいは 'licence()' と入力してください。

R は多くの貢献者による共同プロジェクトです。
詳しくは 'contributors()' と入力してください。
また、R や R のパッケージを出版物で引用する際の形式については
'citation()' と入力してください。

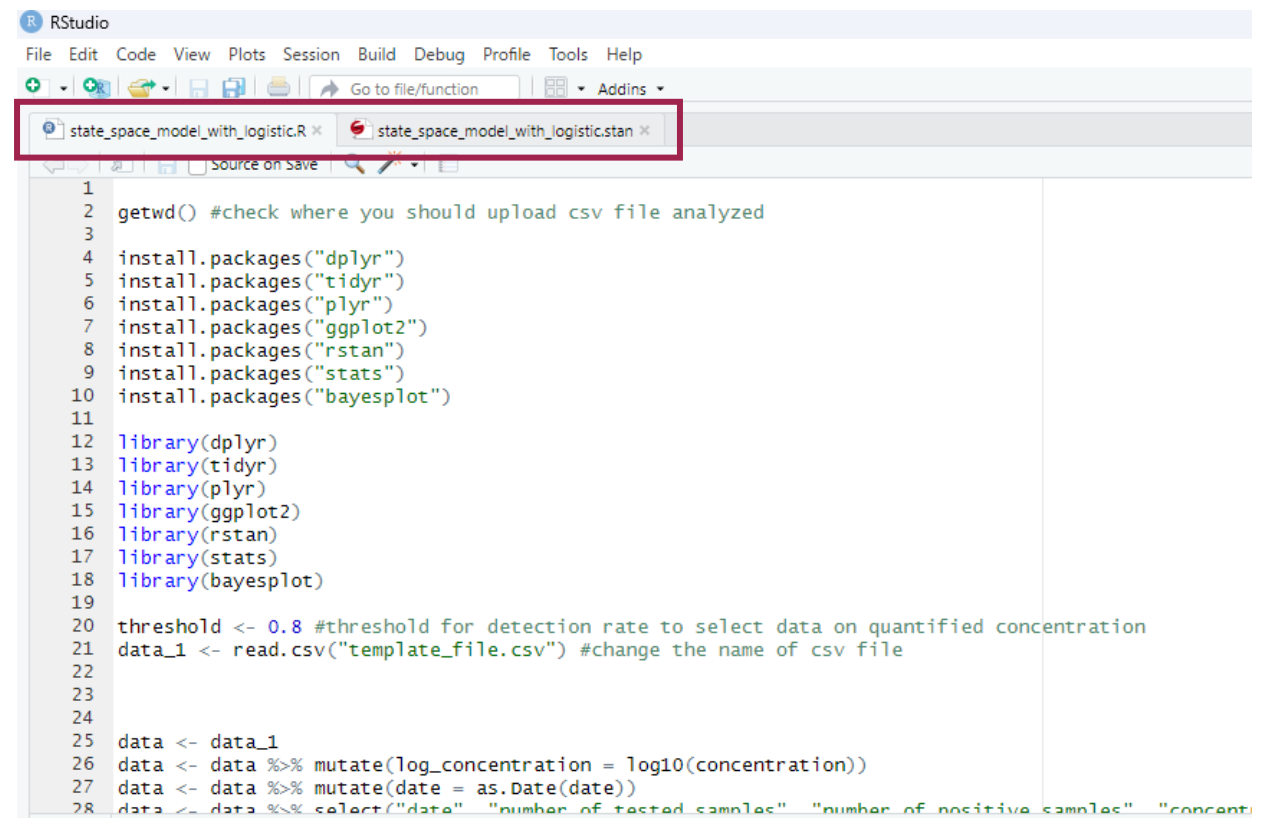
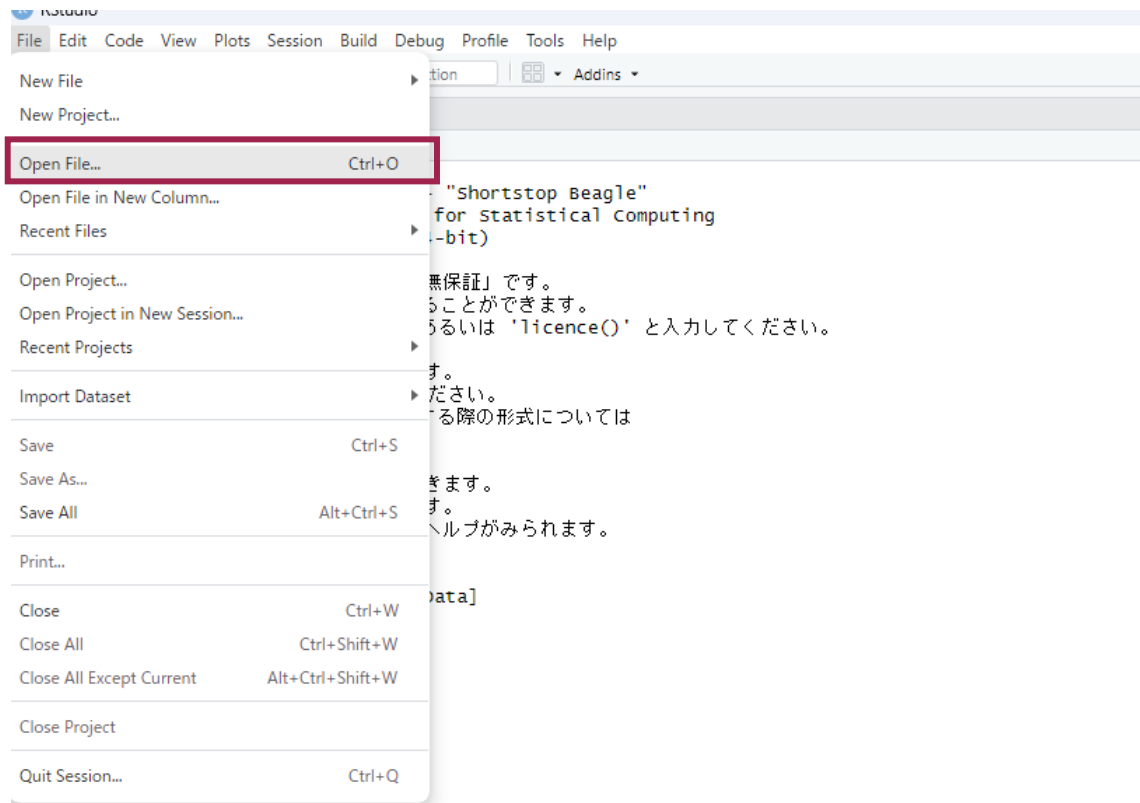
'demo()' と入力すればデモをみるすることができます。
'help()' とすればオンラインヘルプが出ます。
'help.start()' で HTML ブラウザによるヘルプがみられます。
'q()' と入力すれば R を終了します。

[workspace loaded from c:/2023_R/.RData]
> getwd()
[1] "c:/2023_R"
```

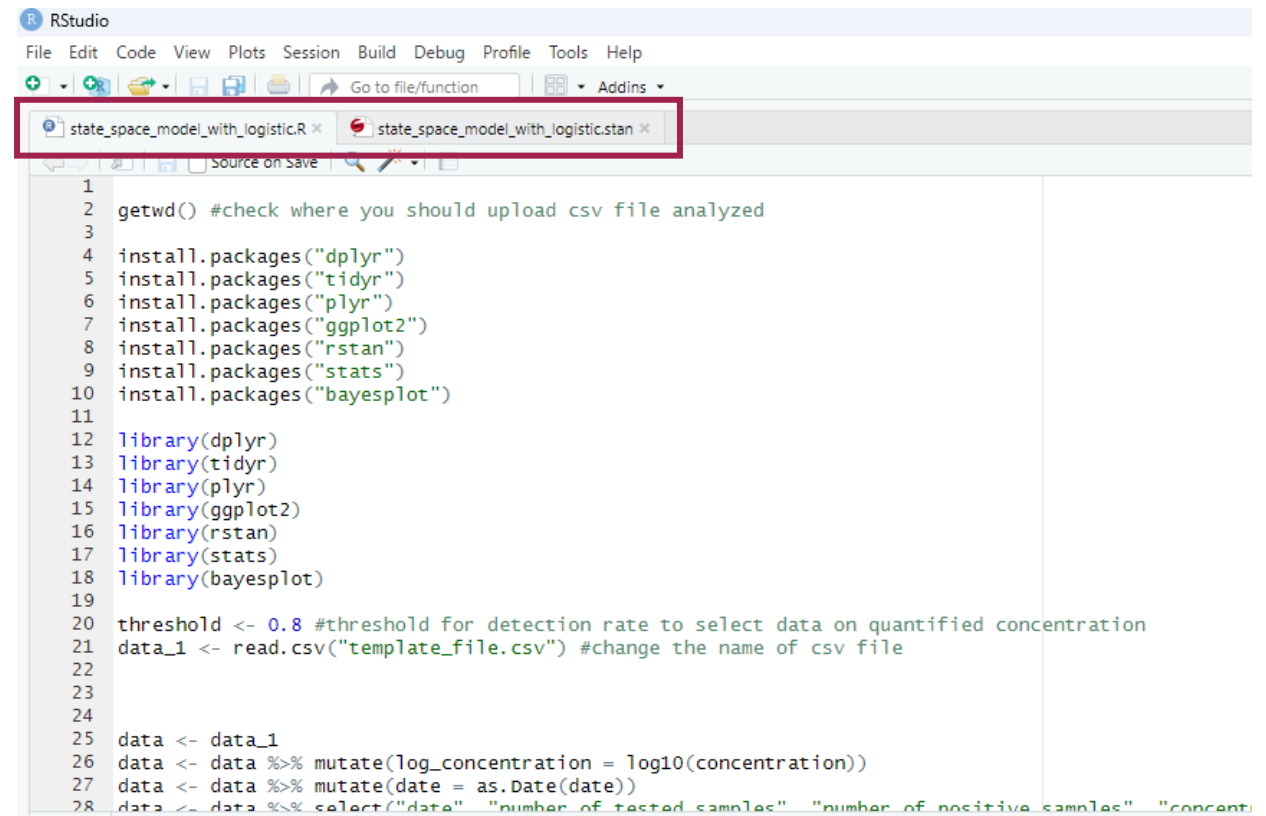
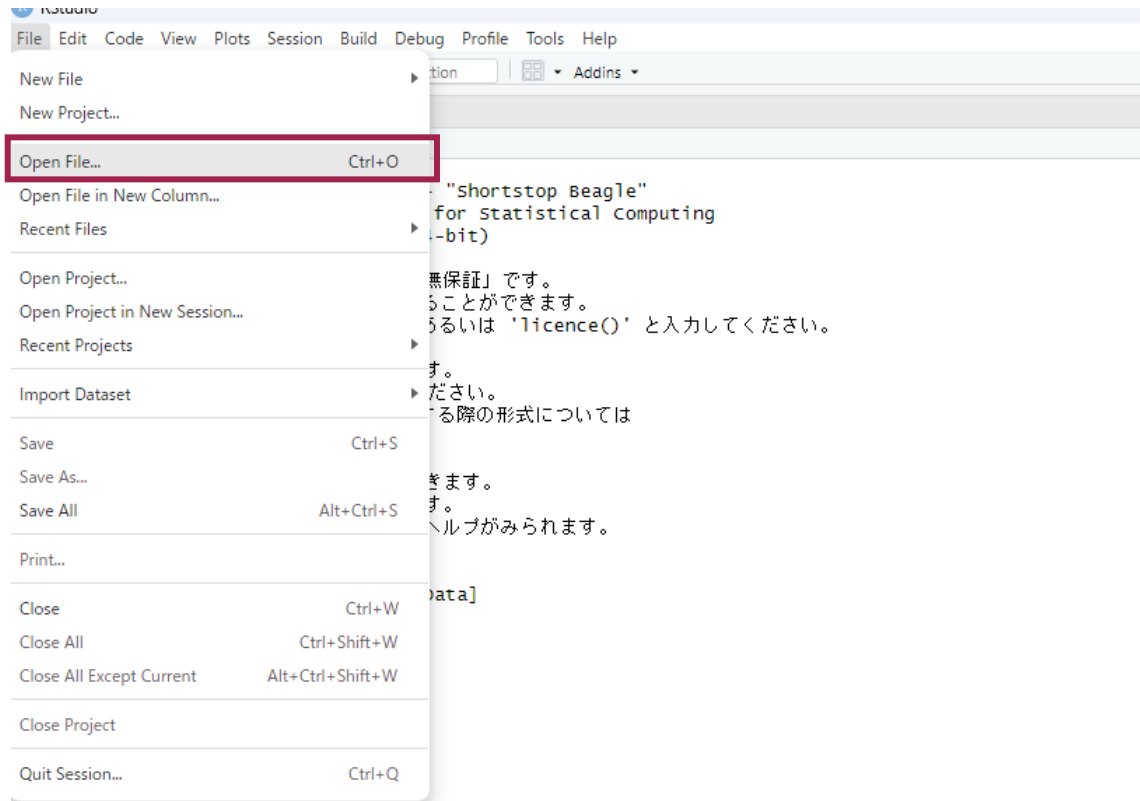
- Type “getwd()”
- In this case, you have to upload the files in “C:/2023_R”

- Drag the files in the “2023_R”

- Open R file and Stan file in Rstudio



- Open R file and Stan file in Rstudio



- Install R packages used in the analysis

The screenshot shows the RStudio interface with a script editor containing R code. The code is as follows:

```
1 getwd() #check where you should upload csv file analyzed
2
3
4 install.packages("dplyr")
5 install.packages("tidyr")
6 install.packages("plyr")
7 install.packages("ggplot2")
8 install.packages("rstan")
9 install.packages("stats")
10 install.packages("bayesplot")
11
12 library(dplyr)
13 library(tidyr)
14 library(plyr)
15 library(ggplot2)
16 library(rstan)
17 library(stats)
18 library(bayesplot)
19
20 threshold <- 0.8 #threshold for detection rate to select data on quantified concentration
21 data_1 <- read.csv("template_file.csv") #change the name of csv file
22
23
24
25 data <- data_1
26 data <- data %>% mutate(log_concentration = log10(concentration))
27 data <- data %>% mutate(date = as.Date(date))
28 data <- data %>% select("date", "number_of_tested_samples", "number_of_positive_samples", "concentration", "log_concentration")
29 colnames(data) <- c("date", "count", "positive", "concentration")
30
31
```

Annotations on the screenshot:

- 1. Drag**: Points to the R logo icon in the top-left corner of the script editor.
- 2. Click**: Points to the **Run** button (a green arrow icon) in the top-right corner of the script editor.

Note: You no longer need to repeat this process once the packages are installed.

- Upload library used in the analysis

RStudio

File Edit Code View Plots Session Build Debug Profile Tools Help

Go to file/function Addins

state_space_model_with_logistic_highs... 20240917_simulation_2_without_round.R Figure_5.R Figure_4.R

Source on Save

1. Drag

```
1  
2 getwd() #check where you should upload csv file analyzed  
3  
4 install.packages("dplyr")  
5 install.packages("tidyr")  
6 install.packages("plyr")  
7 install.packages("ggplot2")  
8 install.packages("rstan")  
9 install.packages("stats")  
10 install.packages("bayesplot")  
11  
12  
13  
14 library(dplyr)  
15 library(tidyr)  
16 library(plyr)  
17 library(ggplot2)  
18 library(rstan)  
19 library(stats)  
20 library(bayesplot)  
21  
22 threshold <- 0.8 #threshold for detection rate to select data on quantified concentration  
23 d <- read.csv("template_file.csv") #change the name of csv file  
24  
25  
26  
27 data <- data_1  
28 data <- data %>% mutate(log_concentration = log10(concentration))  
29 data <- data %>% mutate(date = as.Date(date))  
30 data <- data %>% select("date", "number_of_tested_samples", "number_of_positive_samples", "log_concentration")  
31 colnames(data) <- c("date", "count", "positive", "concentration")  
32  
33  
34  
35 #state-space model with logistic  
36 data_stan <- data  
37 data_stan <- data_stan %>% mutate(positive_rate = positive/count)  
38 sample_size <- nrow(data_stan)  
39
```

2. Click

Run

21:1 (Top Level) R Script

- Set arbitrary threshold (0.7 ~ 1.0)
- Import data

```

1 getwd() #check where you should upload csv file analyzed
2
3
4 install.packages("dplyr")
5 install.packages("tidyr")
6 install.packages("plyr")
7 install.packages("ggplot2")
8 install.packages("rstan")
9 install.packages("stats")
10 install.packages("bayesplot")
11
12 library(dplyr)
13 library(tidyr)
14 library(plyr)
15 library(ggplot2)
16 library(rstan)
17 library(stats)
18 library(bayesplot)
19
20 threshold <- 0.8 #threshold for detection rate to select data on quantified concentration
21 data_1 <- read.csv("template_file.csv") #change the name of csv file

```



Check the name of CSV file you uploaded

```

1 getwd() #check where you should upload csv file analyzed
2
3
4 install.packages("dplyr")
5 install.packages("tidyr")
6 install.packages("plyr")
7 install.packages("ggplot2")
8 install.packages("rstan")
9 install.packages("stats")
10 install.packages("bayesplot")
11
12 library(dplyr)
13 library(tidyr)
14 library(plyr)
15 library(ggplot2)
16 library(rstan)
17 library(stats)
18 library(bayesplot)
19
20 threshold <- 0.8 #threshold for detection rate to select data on quantified concentration
21 data_1 <- read.csv("template_file.csv") #change the name of csv file

```

Console Terminal Background Jobs

R 4.2.3 - C:\WBE\ND\

* See ?bayesplot_theme_set for details on theme setting
警告メッセージ:
パッケージ 'bayesplot' はバージョン 4.3.2 の R の下で壊れました

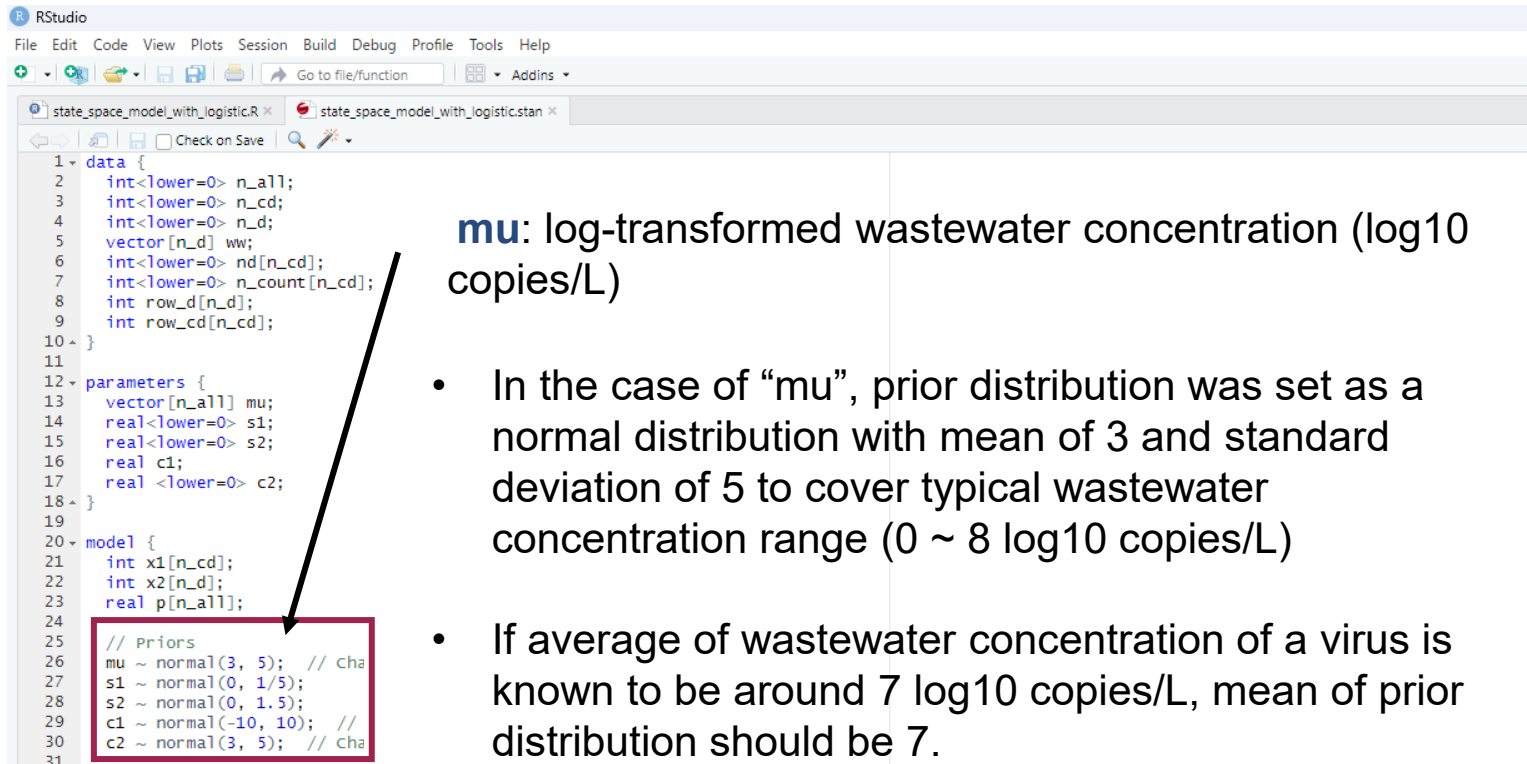
```

> threshold <- 0.8 #threshold for detection rate to select data on quantified concentration
data_1 <- read.csv("template_file.csv") #change the name of csv file
> data_1

```

	date	number_of_tested_samples	number_of_positive_samples	concentration
1	2022/1/1	0	0	NA
2	2022/1/2	0	0	NA
3	2022/1/3	0	0	NA
4	2022/1/4	0	0	NA
5	2022/1/5	0	0	NA
6	2022/1/6	0	0	NA
7	2022/1/7	0	0	NA
8	2022/1/8	2	1	1334.9637
9	2022/1/9	3	3	1842.5722
10	2022/1/10	5	3	2632.2921
11	2022/1/11	5	3	3171.8280
12	2022/1/12	4	3	2149.0025
13	2022/1/13	5	2	4058.2536
14	2022/1/14	4	1	13460.9749
15	2022/1/15	5	1	8864.0000
16	2022/1/16	5	2	3543.9927
17	2022/1/17	5	1	10151.7241
18	2022/1/18	5	1	7078.2516

- Prior distributions are important for convergence of parameters
(Prior distribution should be decided from available information)



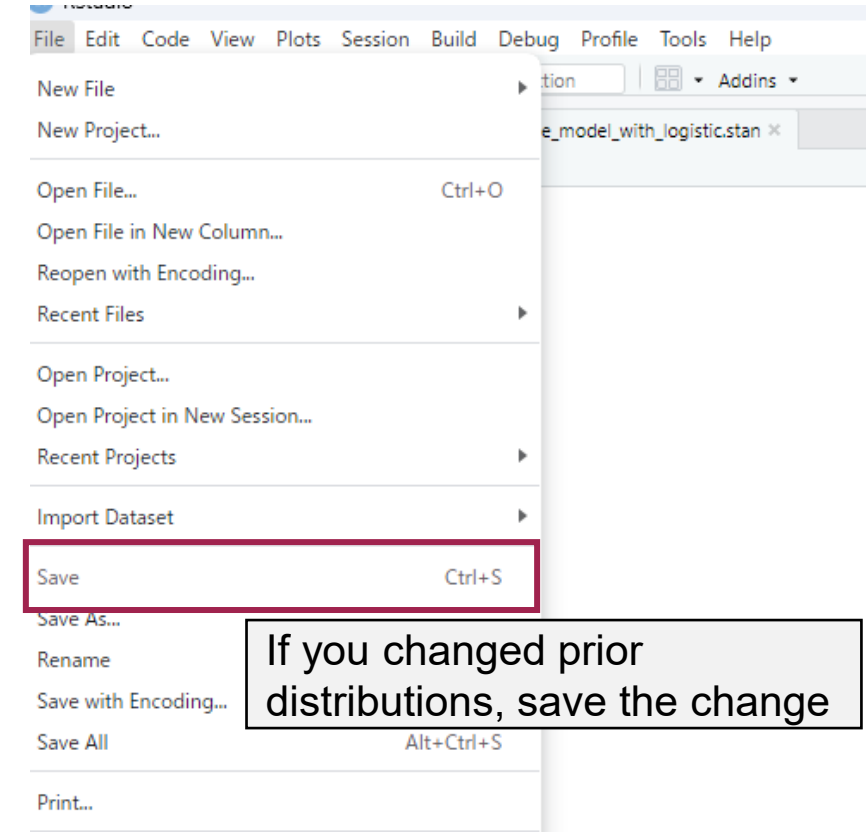
```

1 data {
2   int<lower=0> n_all;
3   int<lower=0> n_cd;
4   int<lower=0> n_d;
5   vector[n_d] ww;
6   int<lower=0> nd[n_cd];
7   int<lower=0> n_count[n_cd];
8   int row_d[n_d];
9   int row_cd[n_cd];
10 }
11
12 parameters {
13   vector[n_all] mu;
14   real<lower=0> s1;
15   real<lower=0> s2;
16   real c1;
17   real <lower=0> c2;
18 }
19
20 model {
21   int x1[n_cd];
22   int x2[n_d];
23   real p[n_all];
24
25   // Priors
26   mu ~ normal(3, 5); // cha
27   s1 ~ normal(0, 1/5);
28   s2 ~ normal(0, 1.5);
29   c1 ~ normal(-10, 10); //
30   c2 ~ normal(3, 5); // cha
31 }

```

mu: log-transformed wastewater concentration (log10 copies/L)

- In the case of “mu”, prior distribution was set as a normal distribution with mean of 3 and standard deviation of 5 to cover typical wastewater concentration range (0 ~ 8 log10 copies/L)
- If average of wastewater concentration of a virus is known to be around 7 log10 copies/L, mean of prior distribution should be 7.



- S_1 is a parameter of the state-formula.
- S_2 is a parameter of the observation formula (i.e., measurement error).
- C_1 and C_2 are parameters of logistic function.

- Drag the row from 25-87 and click Run

```

state_space_model_with_logistic.R x state_space_model_with_logistic.stan x
Source on Save
25 data <- data_1
26 data <- data %>% mutate(log_concentration = log10(concentration))
27 data <- data %>% mutate(date = as.Date(date))
28 data <- data %>% select("date", "number_of_tested_samples", "number_of_positive_samples", "concentration", "log_concentration")
29 colnames(data) <- c("date", "count", "positive", "concentration")
30
31
32
33 #state-space model with logistic
34 data_stan <- data
35 data_stan <- data_stan %>% mutate(positive_rate = positive/count)
36 sample_size <- nrow(data_stan)
37
38 #vector of row number used for the analysis
39 #pick row numbers for censored data
40 data_row_D <- data.frame(true = which((data_stan$positive_rate >= threshold)))
41 sample_size_D <- nrow(data_row_D)
42 #pick row numbers for censored data
43 data_row_CD <- data.frame(true = which(data_stan$count > 0))
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60 mcmc <- stan(
61   file = "state_space_model_with_logistic.stan",
62   data = data_list_ww,
63   seed = 1,
64   chain = 4,
65   iter = 200000,
66   warmup = 100000,
67   thin = 4
68 )
69
70 print(mcmc, pars = c("c1", "c2", "s1", "s2"), probe = c(0.025, 0.50, 0.975))
71
72 #check traceplots if you want
73 #mcmc_combo(mcmc, pars = c("c1", "c2", "s1", "s2"))
74
75
76 #MCMC samples and 95% credible intervals
77 mcmc_sample <- rstan::extract(mcmc)
78 state_name <- "mu"
79 result <- data.frame(t(apply(
80   X = mcmc_sample[[state_name]],
81   MARGIN = 2,
82   FUN = quantile,
83   probs = c(0.025, 0.5, 0.975) #credible interval can be changed
84 )))
85
86 colnames(result) <- c("low", "median", "upr")
87 data_estimated_concentration <- cbind(data, result)

```

MCMC condition can be changed according to your data. (<https://mc-stan.org/rstan/reference/stan.html>)

- Check the convergence of parameters in the state-space model

```
> print(mcmc, pars = c("c1", "c2", "s1", "s2"), probe = c(0.025, 0.50, 0.975))
Inference for Stan model: anon_model.
4 chains, each with iter=4000; warmup=2000; thin=4;
post-warmup draws per chain=500, total post-warmup draws=2000.
```

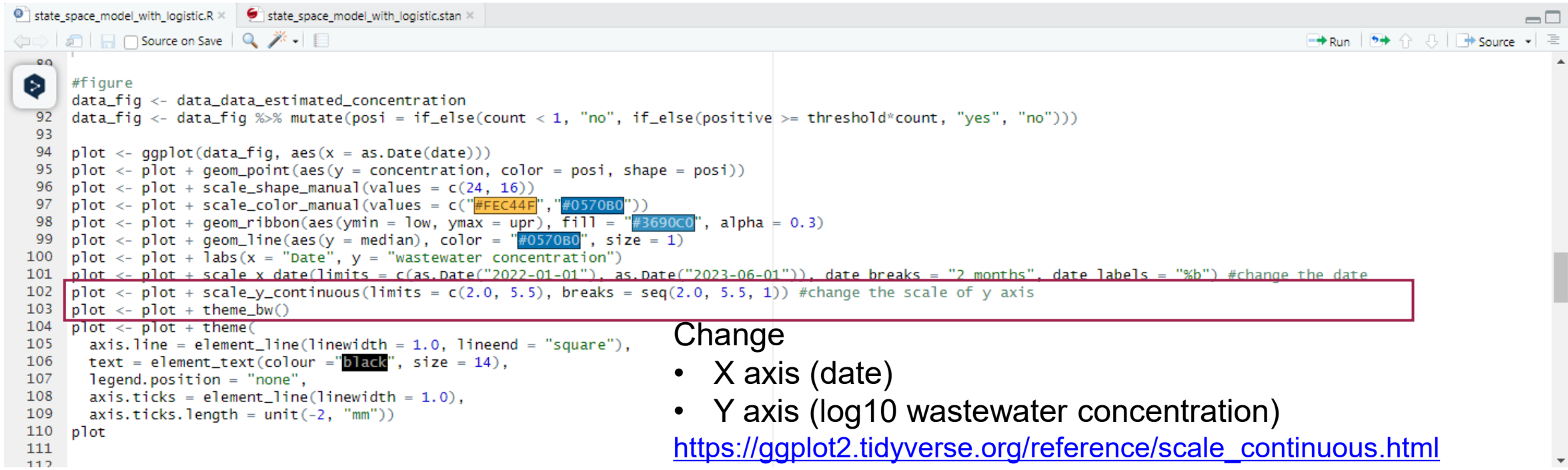
	mean	se_mean	sd	2.5%	25%	50%	75%	97.5%	n_eff	Rhat
c1	-24.55	0.11	3.76	-32.08	-27.04	-24.37	-21.96	-17.60	1208	1.00
c2	8.04	0.03	1.18	5.82	7.21	8.01	8.82	10.39	1565	1.00
s1	0.04	0.00	0.01	0.02	0.03	0.04	0.05	0.07	272	1.02
s2	0.96	0.00	0.15	0.71	0.85	0.94	1.04	1.31	1805	1.00

- Rhat should be lower than 1.10 (<https://mc-stan.org/misc/warnings.html#bulk-ess>)
- N_eff should be higher than 400 (ideally, 1000)

To improve Rhat and n_eff

- Fix prior distribution
- Increase chain, iter (warmup), and thin
- Conduct re-parameterization (**Slide number 14 - 15**)

- Create figures and check the estimation of wastewater concentration



```

#figure
data_fig <- data_data_estimated_concentration
data_fig <- data_fig %>% mutate(posi = if_else(count < 1, "no", if_else(positive >= threshold*count, "yes", "no")))

plot <- ggplot(data_fig, aes(x = as.Date(date)))
plot <- plot + geom_point(aes(y = concentration, color = posi, shape = posi))
plot <- plot + scale_shape_manual(values = c(24, 16))
plot <- plot + scale_color_manual(values = c("#FEC44F", "#0570B0"))
plot <- plot + geom_ribbon(aes(ymin = low, ymax = upr), fill = "#3690C0", alpha = 0.3)
plot <- plot + geom_line(aes(y = median), color = "#0570B0", size = 1)
plot <- plot + labs(x = "Date", y = "wastewater concentration")
plot <- plot + scale_x_date(limits = c(as.Date("2022-01-01"), as.Date("2023-06-01")), date_breaks = "2 months", date_labels = "%b") #change the date
plot <- plot + scale_y_continuous(limits = c(2.0, 5.5), breaks = seq(2.0, 5.5, 1)) #change the scale of y axis
plot <- plot + theme_bw()
plot <- plot + theme(
  axis.line = element_line(linewidth = 1.0, lineend = "square"),
  text = element_text(colour = "black", size = 14),
  legend.position = "none",
  axis.ticks = element_line(linewidth = 1.0),
  axis.ticks.length = unit(-2, "mm"))
plot

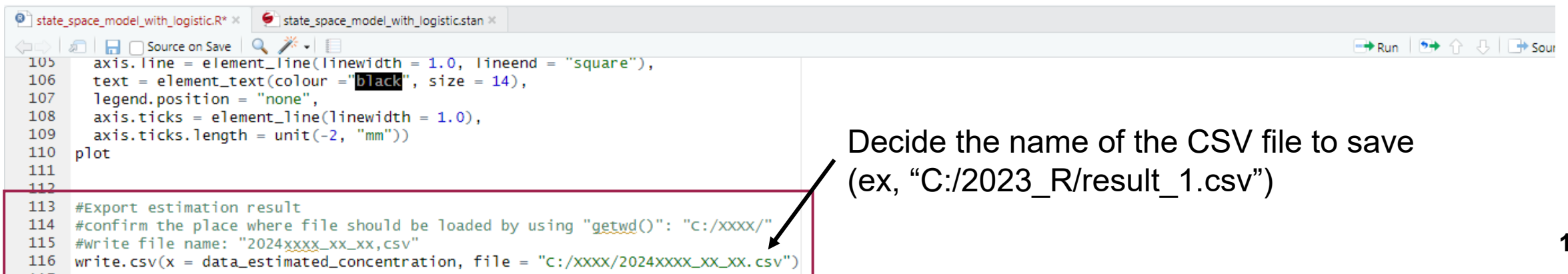
```

Change

- X axis (date)
- Y axis (log10 wastewater concentration)

https://ggplot2.tidyverse.org/reference/scale_continuous.html

- Export the result in CSV file



```

axis.line = element_line(linewidth = 1.0, lineend = "square"),
text = element_text(colour = "black", size = 14),
legend.position = "none",
axis.ticks = element_line(linewidth = 1.0),
axis.ticks.length = unit(-2, "mm"))
plot
#Export estimation result
#confirm the place where file should be loaded by using "getwd()": "c:/xxxx/"
#write file name: "2024xxxx-xx-xx.csv"
write.csv(x = data_estimated_concentration, file = "c:/xxxx/2024xxxx-xx-xx.csv")

```

Decide the name of the CSV file to save
(ex, "C:/2023_R/result_1.csv")

High speed analysis

- The above approach (file name: state_space_model_with_logistic.R & state_space_model_with_logistic.stan) requires a lot of analytical time.
- This problem is solved by using re-parameterization approach.
 - https://mc-stan.org/docs/2_18/stan-users-guide/reparameterization-section.html
 - <https://mc-stan.org/docs/stan-users-guide/reparameterization.html>

202410_WBE_censored_data Private Unwatch

main 2 Branches 0 Tags

Go to file Add file Code

Hiroki-Ando1998 Update state_space_model_with_logistic_highspeed.R 9d79eab · 2 months ago 57 Commits

Analysis of real-world data	Update 20240823_Figure_4_RSV_2_substitution.R	4 months ago
Figure	Add files via upload	4 months ago
Raw data on wastewater concentration of IAV ...	Delete Raw data on wastewater concentration of IAV and RS...	4 months ago
Simulation	Update 20240809_WBE_ND_simulation_1.R	5 months ago
Protocol for the state_space_model.pdf	Add files via upload	4 months ago
state_space_model_with_logistic.R	Update state_space_model_with_logistic.R	3 months ago
state_space_model_with_logistic.stan	Add files via upload	4 months ago
state_space_model_with_logistic_highspeed.R	Update state_space_model_with_logistic_highspeed.R	2 months ago
state_space_model_with_logistic_highspeed.stan	Update state_space_model_with_logistic_highsp...	2 months ago
template_example_file.xlsx	Add files via upload	4 months ago
template_file.csv	Add files via upload	4 months ago

Hiroki-Ando1998 / 202410_WBE_censored_data

Code Issues Pull requests Actions Projects Security Insights Settings

Files

main + Go to file

202410_WBE_censored_data / state_space_model_with_logistic_highspeed.stan in main

Edit Preview Code 55% faster with GitHub Copilot

```

53 data_nd <- data_stan %>% filter(count > 0)
54 ND <- data_nd$positive
55 count <- data_nd$count
56
57 data_list_vw <- list(n_all = sample_size, n_cd = sample_size_CD, n_d = sample_size_D,
58                    vw = vw, nd = ND, row_cd = data_row_CD$true, row_d = data_row_D$true, n_count = count)
59
60 rstan_options(auto_write = TRUE)
61 options(mc.cores = parallel::detectCores())
62
63 mcmc <- stan(
64   file = "state_space_model_with_logistic_highspeed.stan",
65   data = data_list_vw,
66   seed = 1,
67   chain = 4,
68   iter = 10000,
69   warmup = 5000,
70   thin = 4
71 )
72
73 print(mcmc, pars = c("c1", "c2", "s1", "s2"), probe = c(0.025, 0.50, 0.975))

```

R file is same, except for this line.

High speed analysis

The purpose of reparameterization is to standardize the scale of the prior distributions so that the sampling space becomes narrower and more isotropic, allowing the sampler to explore the parameter space more efficiently.

state_space_model_with_logistic_highspeed.stan (Stan file)

```
12 parameters {
13   vector<lower=-4, upper=4>[n_all] mu_raw;
14   real<lower=-4, upper=4> s1_raw;
15   real<lower=-4, upper=4> s2_raw;
16   real<lower=-4, upper=4> c1_raw;
17   real<lower=-4, upper=4> c2_raw;
18 }
```

Range of parameters

```
19
20 transformed parameters {
21   vector[n_all] mu;
22   for (i in 1:n_all) {
23     mu[i] = 3.5 + 1.5 * mu_raw[i];
24   }
25   real s1;
26   s1 = exp(s1_raw - 2);
27
28   real s2;
29   s2 = exp(s2_raw - 2);
30
31   real c1;
32   c1 = -22 + 5*c1_raw;
33
34   real c2;
35   c2 = 6 + 3*c2_raw;
36
37 }
```

Parameters are converted into reasonable scale values, which is expected from previous studies.

- In this case, typical range of wastewater concentration is expected to be 0.5 to 6.5 \log_{10} copies/L.
- Typically, S_1 and S_2 are positive values, ranging from 0 to 1.
- C_1 and C_2 are probably in this range, according to a previous study.

These values can be changed, according to your dataset.
(Do not forget to save file after changing values.)

```
39
40 model {
41   // Priors
42   mu_raw ~ normal(0, 1);
43   s1_raw ~ normal(0, 1);
44   s2_raw ~ normal(0, 1);
45   c1_raw ~ normal(0, 1);
46   c2_raw ~ normal(0, 1);
47
48   // Autoregressive prior for mu
49   mu[3:n_all] ~ normal(2 * mu[2:n_all-1] - mu[1:n_all-2], s1);
50 }
```

The same prior distribution



- Run MCMC sampling from R file
- Check R-hat and n_eff
- Confirm estimated wastewater concentrations.