

# Model analysis

## Non Linear Dynamics

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## LAC Operon Model analysis

Based on Yildirim et al. 2004.

See repository for more information.

### Setup

```
library(tidyverse)

## -- Attaching packages ----- tidyverse 1.3.1 --
## v ggplot2 3.3.6      v purrr   0.3.4
## v tibble  3.1.7      v dplyr   1.0.9
## v tidyr   1.2.0      v stringr 1.4.0
## v readr   2.1.2      v forcats 0.5.1

## -- Conflicts ----- tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()     masks stats::lag()

library(broom)
options(scipen=999)
```

### Models with one starting condition

#### Loading simulation results

Loading data into dataframes

```
original = read_csv("results/Original model 2022-11-11 02:41:58.csv")
corrected = read_csv("results/Corrected model 2022-11-11 02:42:02.csv")
```

Combining into one DF

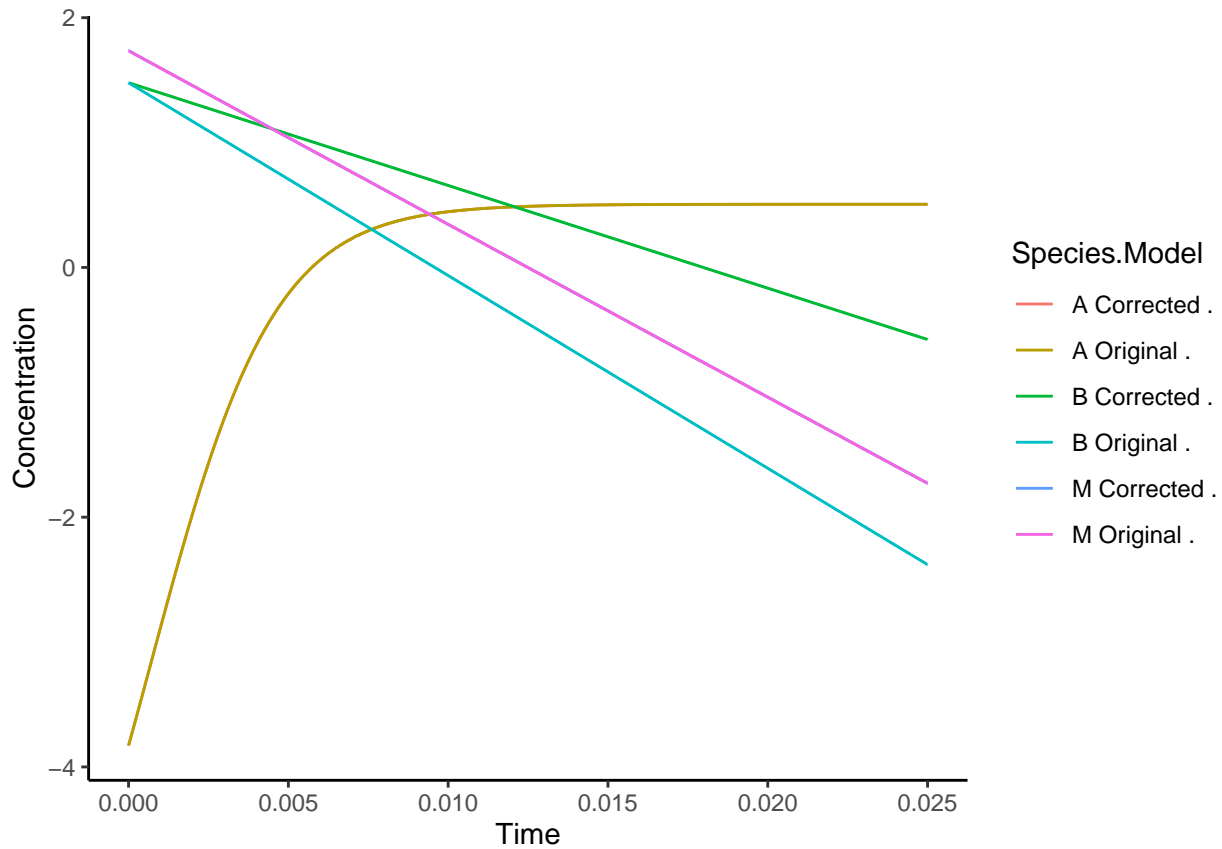
```
data <-
  bind_rows(original %>% mutate(Model = "Original"), corrected %>% mutate(Model = "Corrected"))
```

Scaling and pivoting data

```
data <-
  data %>%
  mutate(across(-c(Time, Model), scale)) %>%
  pivot_longer(cols = -c(Time, Model), names_to="Species", values_to="Concentration") %>%
  mutate(across(c(Model, Species), as.factor))
```

## Visualising results

```
ggplot(data %>% mutate(Species.Model = paste(Species, Model, delimiter=".")), aes(x=Time, y=Concentration)) +  
  geom_line() +  
  #scale_y_log10() +  
  theme_classic()
```



## Model analysis

Checking hypothesis: There is no significant difference between the data measured with either model.

```
data %>%  
  group_by(Species) %>%  
  nest() %>%  
  mutate(F_test = map(data, ~ aov(Concentration ~ Model + Time, data = .x) %>% tidy() %>% pluck("p.value")) %>%  
  unnest(F_test) %>%  
  select(-data)
```

```
## # A tibble: 3 x 2  
## # Groups:   Species [3]  
##   Species F_test  
##   <fct>    <dbl>  
## 1 M        0.916  
## 2 B         0  
## 3 A        1.00
```

## Models with a scan of starting conditions

### Loading simulation results

Loading data into dataframes

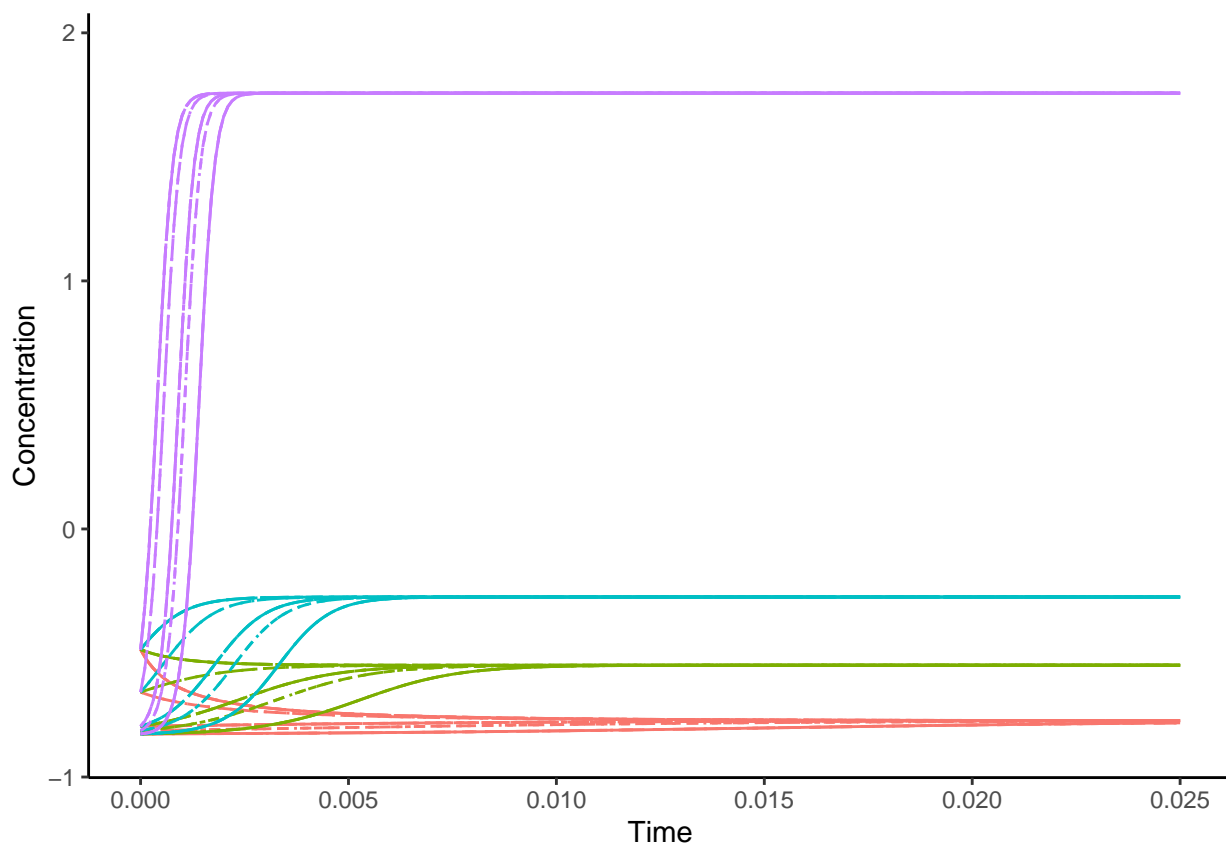
```
data <- read_csv("results/Starting conditions scan 2022-11-11 10:37:22.csv") %>%  
  mutate(across(c(Model, Starting_Conditions_Set, L), as.factor))
```

Scaling and pivoting data

```
pivot_scaled_data <-  
  data %>%  
  mutate(across(c(M, B, A), scale)) %>%  
  pivot_longer(cols = -c(Time, Model, Starting_Conditions_Set, L), names_to="Species", values_to="Concentration") %>%  
  mutate(across(c(Species), as.factor))
```

### Visualising results

```
ggplot(pivot_scaled_data %>% filter(Model == "Corrected") %>% mutate(Species.Set = paste(Species, Starting_Conditions_Set)) %>%  
  geom_line(show.legend=F) +  
  #scale_y_log10() +  
  theme_classic()
```



```
sim_end = max(data$Time)  
data %>%  
  pivot_longer(cols=c(M, B, A), names_to="Species", values_to="Concentration") %>%  
  filter(Time == sim_end) %>%  
  group_by(Species, L) %>%
```

```
summarize(SteadyState=mean(Concentration))
```

```
## `summarise()` has grouped output by 'Species'. You can override using the
## `.groups` argument.
```

```
## # A tibble: 12 x 3
## # Groups:   Species [3]
##   Species L      SteadyState
##   <chr>    <fct>         <dbl>
## 1 A      10000      15876.
## 2 A      50000      81515.
## 3 A     100000     161539.
## 4 A     500000     752458.
## 5 B      10000         6.62
## 6 B      50000         6.62
## 7 B     100000         6.62
## 8 B     500000         6.62
## 9 M      10000        11.5
## 10 M     50000        11.5
## 11 M     100000        11.5
## 12 M     500000        11.5
```

## Model analysis

Checking hypothesis: There is no significant difference between the data measured with either model.

```
pivot_scaled_data %>%
  group_by(Species) %>%
  nest() %>%
  mutate(F_test = map(data, ~ aov(Concentration ~ Model + Time + L + Starting_Conditions_Set, data = .x))
  unnest(F_test)
```

```
## # A tibble: 3 x 3
## # Groups:   Species [3]
##   Species data          F_test
##   <fct>    <list>         <dbl>
## 1 M      <tibble [251,000 x 5]>  1.00
## 2 B      <tibble [251,000 x 5]>   0
## 3 A      <tibble [251,000 x 5]>  1.00
```