Lab Notebook: Theophylline Data and Models

CTSI Symposium

2024-02-26

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> **ℹ Note**
>
> To render a pdf or word document update your header text to:
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> **💡 Reference for YAML Header**
>
> List of Quarto output options: https://r4ds.hadley.nz/quarto-formats
> List of header options: https://cran.r-project.org/web/packages/ymlthis/vignettes/yaml-fieldguide.html

1 Notebook 1

Start Date: February 28th 2024

End Date: …

1.1 Introduction

Theophylline is a medication used to treat asthma and chronic obstructive pulmonary disease as a second-line drug. It is a bronchodilator. This activity reviews the indications, action, and contraindications for theophylline as a potential agent in treating asthma and chronic obstructive pulmonary disease. This activity will highlight the mechanism of action, adverse event profile, pharmacokinetics, and drug interactions pertinent for members of the interprofessional team in the treatment of patients with asthma and chronic obstructive pulmonary disease. (https://www.ncbi.nlm.nih.gov/books/NBK519024/). The chemical structure (Figure 1) is shown below:

1.2 Goals
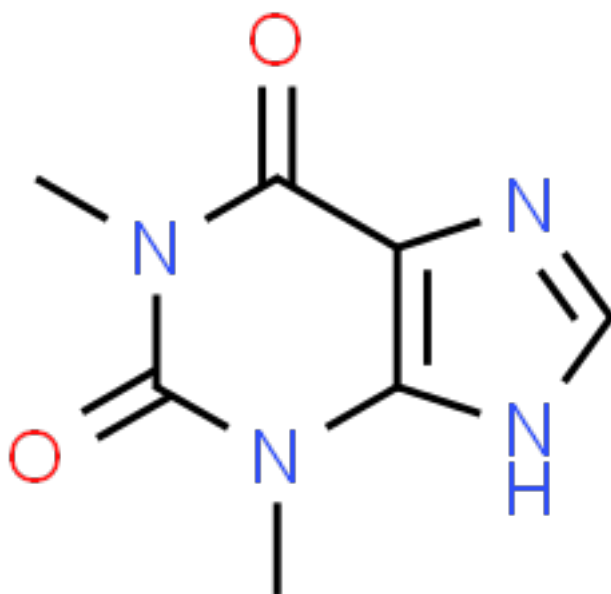
Develop a PopPK model for theophylline.

Figure 1: Chemical Structure

1.3 Raw Data

```r
library(ggplot2)
data<-Theoph

ggplot(data=Theoph, aes(x=Time, y=conc, color=as.factor(Subject)))+
  geom_point(size=4)+
  geom_line()+
  labs(y="Concentration (mg/L)", x="Time (hrs)")+
  guides(color="none",
         element_text(size=10))+
  theme_bw()
```
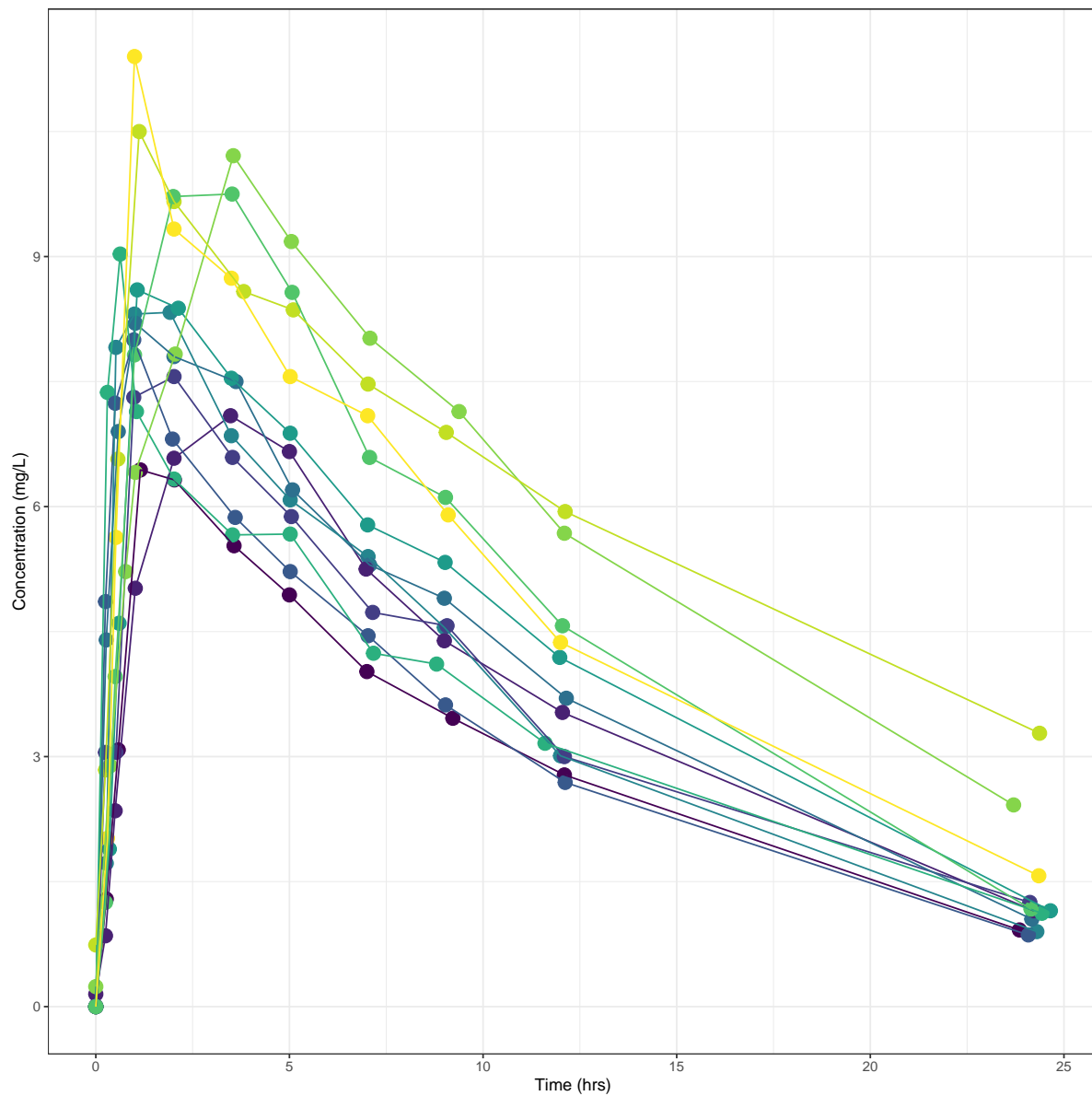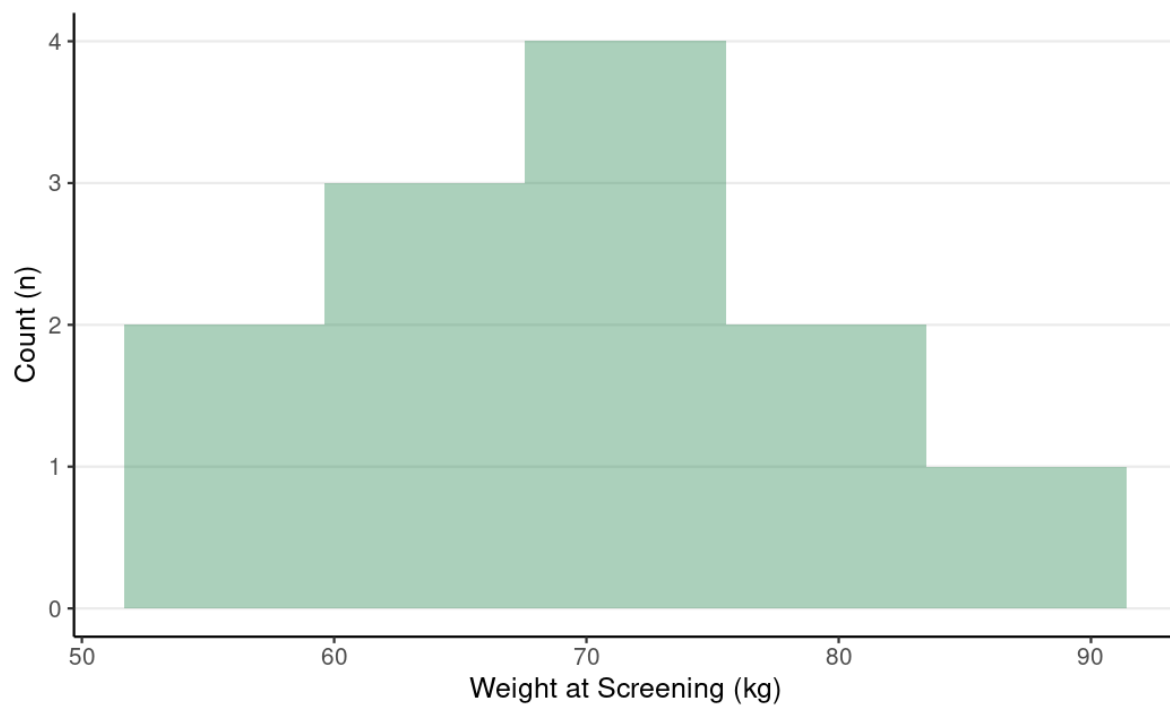
Figure 2: Theoph PK Profile

As shown in Figure 2 we have 12 IDs with PK data collected over 25 hours. The only other covariate we have is weight and that is plotted below in Figure 3.

```{r}
#| tbl-cap: "Theoph PK summary"
#| label: tbl-PK-sum
```

Figure 3: Histogram of Subject's Weight

```
data%>%
  mutate(Time=as.numeric(Time))%>%
  mutate(Time=round(Time, digits = 1))%>%
  group_by(Time)%>%
  mutate(DV=median(conc))%>%
  dplyr::select(Time,DV)%>%
  ungroup()%>%
  unique()%>%
  arrange(desc(-Time))%>%
gt()
```

Table 1: Theoph PK summary

Time	DV
0.0	0.000
0.2	2.840
0.3	1.955
0.4	2.890
0.5	4.795
0.6	6.570
0.8	5.220
1.0	7.820
1.1	8.600
1.9	8.330
2.0	7.680
2.1	8.380
3.5	7.315
3.6	5.870
3.8	8.580
5.0	6.080
5.1	8.360
7.0	5.400
7.1	6.590
7.2	4.485
8.8	4.110
9.0	4.725
9.1	5.900
9.2	3.460
9.4	7.140
11.6	3.160

12.0	4.190
12.1	3.530
12.2	3.700
23.7	2.420
23.9	0.920
24.1	1.170
24.2	1.100
24.3	0.900
24.4	1.570
24.6	1.150