# data manipulation hands-on

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```
library(PKPDmisc)
library(readr)
library(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
```

```
library(knitr)
library(ggplot2)
```

## DATA IMPORT

Objectives:

- Import datasets and documents
- Perform basic data manipulation upon importing the data.

### Task-I

Use the .csv files `demog`, `IV`, and `Oral` provided into the data object folder.

1. Read in all three csv files

```
iv_raw <- read_csv("../data/IV.csv")
oral_raw <- read_csv("../data/ORAL.csv")
demog_raw <- read_csv("../data/demog.csv")
```

```
iv_raw %>% head %>% kable
```

| ID | TIME | DV | AMT | DOSE |
|---|---|---|---|---|
| 1 | 0.00 | NA | 100 | 100 |
| 1 | 0.25 | 1273.5 | NA | 100 |
| 1 | 0.50 | 995.38 | NA | 100 |
| 1 | 1.00 | 1254.7 | NA | 100 |
| 1 | 2.00 | 1037.6 | NA | 100 |
| 1 | 3.00 | 1135.4 | NA | 100 |

```
oral_raw %>% head %>% kable
```

| ID | TIME | DV | AMT | DOSE |
|---|---|---|---|---|
| 1 | 0.00 | NA | 100 | 100 |
| 1 | 0.25 | 206.29 | NA | 100 |
| 1 | 0.50 | 514.88 | NA | 100 |
| 1 | 1.00 | 602 | NA | 100 |
| 1 | 2.00 | 1051.2 | NA | 100 |
| 1 | 3.00 | 1021.5 | NA | 100 |

```
demog_raw %>% head %>% kable
```

| ID | SEX | WT | AGE | RACE |
|---|---|---|---|---|
| 1 | Female | 56.8 | 28 | Hispanic |
| 2 | Female | 58.5 | 30 | Black |
| 3 | Male | 69.0 | 48 | Black |
| 4 | Female | 54.8 | 50 | Asian |
| 5 | Male | 78.1 | 35 | Caucasian |
| 6 | Male | 67.4 | 34 | Hispanic |

## DATA MANIPULATION

The goals of this section:

- Use data manipulation tools to prepare the dataset for analysis

### Task-II

1. Add a Formulation column and label IV/Oral for each dataset

```
iv <- iv_raw %>% mutate(FORM = "IV")
oral <- oral_raw %>% mutate(FORM = "ORAL")
```

2. Create one integrated dataset with both IV and Oral data.
3. Rename "DV" column as "COBS"

```
pkdat <- bind_rows(iv, oral) %>% rename(COBS = DV)
```

4. Appropriately merge the demographics dataset into the IV and Oral dataset

Individuals only found in PK:

```
anti_join(pkdat, demog_raw)
```

```
## Joining, by = "ID"
```

```
## # A tibble: 0 × 6
## # ... with 6 variables: ID <int>, TIME <dbl>, COBS <chr>, AMT <int>,
## #   DOSE <int>, FORM <chr>
```

Individuals found only in demographics:

```
anti_join(demog_raw, pkdat)
```

```
## Joining, by = "ID"
```

```
## # A tibble: 2 × 5
##      ID    SEX    WT   AGE      RACE
##   <int>  <chr> <dbl> <int>     <chr>
## 1    52 Female    70    33     Asian
## 2    51   Male    60    28 Caucasian
```

Given missing PK information, we will only retain individuals that also have PK data

```
pkdemog <- left_join(pkdat, demog_raw)
```

```
## Joining, by = "ID"
```

```
pkdemog %>% head %>% kable
```

| ID | TIME | COBS | AMT | DOSE | FORM | SEX | WT | AGE | RACE |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.00 | NA | 100 | 100 | IV | Female | 56.8 | 28 | Hispanic |
| 1 | 0.25 | 1273.5 | NA | 100 | IV | Female | 56.8 | 28 | Hispanic |
| 1 | 0.50 | 995.38 | NA | 100 | IV | Female | 56.8 | 28 | Hispanic |
| 1 | 1.00 | 1254.7 | NA | 100 | IV | Female | 56.8 | 28 | Hispanic |
| 1 | 2.00 | 1037.6 | NA | 100 | IV | Female | 56.8 | 28 | Hispanic |
| 1 | 3.00 | 1135.4 | NA | 100 | IV | Female | 56.8 | 28 | Hispanic |

5. Perform the following tasks:
    a. Ensure that the following columns are numeric and not text: TIME, COBS, WT, AGE, AMT and DOSEs
    b. Change the following:
    c. fix COBS to be numeric
    d. Filter the dataset such that you remove all rows that were non-numeric
    e. Create a new column called "GENDER" where:
        i. Female = 0
        ii. Male = 1
    f. Create a new column called RACEN where:
        i. Caucasian = 0
        ii. Asian = 1
        iii. Black = 2
        iv. Hispanic = 3

```
str(pkdemog)
```

```
## Classes 'tbl_df', 'tbl' and 'data.frame':    1200 obs. of  10 variables:
##  $ ID  : int  1 1 1 1 1 1 1 1 1 1 ...
##  $ TIME: num  0 0.25 0.5 1 2 3 4 6 8 12 ...
##  $ COBS: chr  NA "1273.5" "995.38" "1254.7" ...
##  $ AMT : int  100 NA NA NA NA NA NA NA NA NA ...
##  $ DOSE: int  100 100 100 100 100 100 100 100 100 100 ...
##  $ FORM: chr  "IV" "IV" "IV" "IV" ...
##  $ SEX : chr  "Female" "Female" "Female" "Female" ...
##  $ WT  : num  56.8 56.8 56.8 56.8 56.8 56.8 56.8 56.8 56.8 56.8 ...
##  $ AGE : int  28 28 28 28 28 28 28 28 28 28 ...
##  $ RACE: chr  "Hispanic" "Hispanic" "Hispanic" "Hispanic" ...
```

```
pkdemog <- pkdemog %>%
  mutate(
    NNFLG = ifelse(is.na(COBS), 0,
                   ifelse(!is.na(as.numeric(COBS)), 0, 1))
```

```
  )
```

```
## Warning in ifelse(!is.na(as.numeric(c(NA, "1273.5", "995.38", "1254.7", :
## NAs introduced by coercion
```

```
pkdemog %>% filter(NNFLG == 1) %>% kable()
```

| ID | TIME | COBS | AMT | DOSE | FORM | SEX | WT | AGE | RACE | NNFLG |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | 24 | BQL | NA | 100 | IV | Male | 80.9 | 31 | Asian | 1 |
| 20 | 24 | BQL | NA | 100 | ORAL | Male | 80.9 | 31 | Asian | 1 |

```
pkdemog_cleaned <- pkdemog %>%
  filter(NNFLG == 0) %>%
  mutate(COBS = as_numeric(COBS))
```

6. Save the above modifications as a new csv file, dropping the columns SEX and RACE

```
write_nonmem(pkdemog_cleaned, "../data/pkdemog_cleaned.csv")
```

## Descriptive Statistics

Objectives

- How to make summaries of the data using descriptive statistics and other data manipulation tools (dplyr, base R functions etc)

### Task III

1. Summarize counts stratified by gender and race

```
count(pkdemog_cleaned %>% distinct(ID, .keep_all = T), SEX, RACE) %>% kable()
```

| SEX | RACE | n |
|---|---|---|
| Female | Asian | 4 |
| Female | Black | 6 |
| Female | Caucasian | 13 |
| Female | Hispanic | 5 |
| Male | Asian | 4 |
| Male | Black | 6 |
| Male | Caucasian | 4 |
| Male | Hispanic | 8 |

2. Add a column with the count the number of males/females in the dataset

```
gender_counts <- pkdemog_cleaned %>%
  distinct(ID, .keep_all=TRUE) %>%
  group_by(SEX) %>%
  summarize(CNTGEN = n())

pkdemog_cleaned %>% left_join(gender_counts) %>%
  distinct(ID, .keep_all = T) %>%
  head %>% kable()
```

```
## Joining, by = "SEX"
```

| ID | TIME | COBS | AMT | DOSE | FORM | SEX | WT | AGE | RACE | NNFLG | CNTGEN |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | NA | 100 | 100 | IV | Female | 56.8 | 28 | Hispanic | 0 | 28 |
| 2 | 0 | NA | 100 | 100 | IV | Female | 58.5 | 30 | Black | 0 | 28 |
| 3 | 0 | NA | 100 | 100 | IV | Male | 69.0 | 48 | Black | 0 | 22 |
| 4 | 0 | NA | 100 | 100 | IV | Female | 54.8 | 50 | Asian | 0 | 28 |
| 5 | 0 | NA | 100 | 100 | IV | Male | 78.1 | 35 | Caucasian | 0 | 22 |
| 6 | 0 | NA | 100 | 100 | IV | Male | 67.4 | 34 | Hispanic | 0 | 22 |

4. summarize the min, mean, and max values for WT, AGE:
    a. non-stratified (WT only)
    b. by Gender

```
pkdemog_cleaned %>%
  summarize(minWT = min(WT),
            meanWT = mean(WT),
            maxWT = max(WT))
```

```
## # A tibble: 1 × 3
##   minWT   meanWT maxWT
##   <dbl>    <dbl> <dbl>
## 1  52.3 64.06795  80.9
```

```
pkdemog_cleaned %>%
  group_by(SEX) %>%
  summarize_at(vars(AGE, WT), funs(min, mean, max)) %>% kable()
```

| SEX | AGE_min | WT_min | AGE_mean | WT_mean | AGE_max | WT_max |
|---|---|---|---|---|---|---|
| Female | 20 | 52.3 | 36.96429 | 59.45714 | 51 | 69.0 |
| Male | 28 | 64.3 | 40.49049 | 69.95856 | 59 | 80.9 |

5. Calculate the Median, 5th, and 95th percentile concentration at each time point for each formulation and dose level. hint: you can use `?quantile` to calculate various quantiles

```
quantile_summaries <- pkdemog_cleaned %>% filter(!is.na(COBS)) %>%
  group_by(FORM, DOSE, TIME) %>%
  summarize(q05 = quantile(COBS, 0.05),
            q50 = quantile(COBS, 0.5),
            q95 = quantile(COBS, 0.95))

quantile_summaries %>% kable()
```

| FORM | DOSE | TIME | q05 | q50 | q95 |
|---|---|---|---|---|---|
| IV | 100 | 0.25 | 822.818000 | 1715.6000 | 2750.6600 |
| IV | 100 | 0.50 | 999.604000 | 1536.9000 | 2815.1400 |
| IV | 100 | 1.00 | 1071.120000 | 1422.6000 | 2629.3800 |
| IV | 100 | 2.00 | 750.034000 | 1215.9000 | 1979.6400 |
| IV | 100 | 3.00 | 789.454000 | 1059.2000 | 1802.8400 |
| IV | 100 | 4.00 | 560.956000 | 909.4700 | 1277.5800 |
| IV | 100 | 6.00 | 356.112000 | 695.9600 | 1014.3740 |
| IV | 100 | 8.00 | 174.490000 | 528.9600 | 810.1720 |
| IV | 100 | 12.00 | 79.720000 | 280.4500 | 462.8960 |

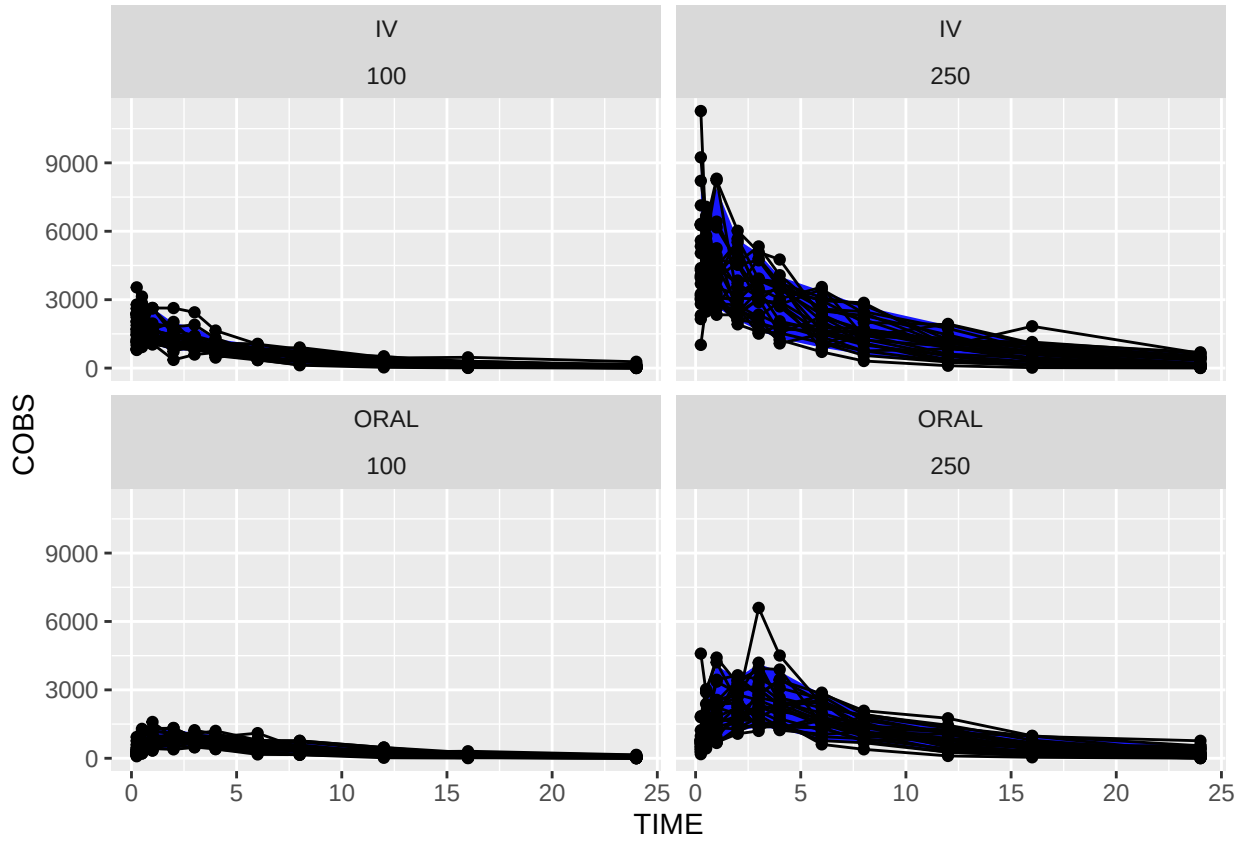
| FORM | DOSE | TIME | q05 | q50 | q95 |
|---|---|---|---|---|---|
| IV | 100 | 16.00 | 19.021600 | 153.9800 | 302.8760 |
| IV | 100 | 24.00 | 3.807910 | 55.0940 | 169.2525 |
| IV | 250 | 0.25 | 2184.120000 | 4292.5000 | 9036.4400 |
| IV | 250 | 0.50 | 2680.400000 | 4720.8000 | 6643.0600 |
| IV | 250 | 1.00 | 2657.800000 | 3892.5000 | 7872.3200 |
| IV | 250 | 2.00 | 2096.660000 | 3062.7000 | 5637.6800 |
| IV | 250 | 3.00 | 1644.920000 | 3096.2000 | 5029.8600 |
| IV | 250 | 4.00 | 1300.120000 | 2928.6000 | 4014.5600 |
| IV | 250 | 6.00 | 894.444000 | 1837.5000 | 3379.0200 |
| IV | 250 | 8.00 | 593.554000 | 1532.7000 | 2700.6400 |
| IV | 250 | 12.00 | 254.336000 | 961.4400 | 1871.9800 |
| IV | 250 | 16.00 | 127.992000 | 617.0800 | 1133.0000 |
| IV | 250 | 24.00 | 16.746000 | 138.3200 | 644.1220 |
| ORAL | 100 | 0.25 | 116.238000 | 243.9600 | 729.1820 |
| ORAL | 100 | 0.50 | 219.358000 | 418.8000 | 1095.5180 |
| ORAL | 100 | 1.00 | 356.370000 | 613.1500 | 1288.1000 |
| ORAL | 100 | 2.00 | 459.004000 | 850.0400 | 1283.4600 |
| ORAL | 100 | 3.00 | 504.412000 | 733.0300 | 1096.0600 |
| ORAL | 100 | 4.00 | 417.484000 | 779.8000 | 1037.5400 |
| ORAL | 100 | 6.00 | 249.916000 | 511.2300 | 823.0760 |
| ORAL | 100 | 8.00 | 156.652000 | 434.4900 | 754.0580 |
| ORAL | 100 | 12.00 | 69.605600 | 235.0000 | 461.8440 |
| ORAL | 100 | 16.00 | 22.982000 | 131.5400 | 237.3840 |
| ORAL | 100 | 24.00 | 4.061125 | 43.5375 | 129.3972 |
| ORAL | 250 | 0.25 | 275.032000 | 709.5700 | 1837.4600 |
| ORAL | 250 | 0.50 | 522.846000 | 1152.3000 | 2785.5800 |
| ORAL | 250 | 1.00 | 703.254000 | 1824.5000 | 4055.5800 |
| ORAL | 250 | 2.00 | 1194.720000 | 2307.1000 | 3532.7200 |
| ORAL | 250 | 3.00 | 1362.160000 | 2366.9000 | 4142.9800 |
| ORAL | 250 | 4.00 | 1269.500000 | 2248.5000 | 3805.1200 |
| ORAL | 250 | 6.00 | 807.978000 | 1771.1000 | 2807.2200 |
| ORAL | 250 | 8.00 | 695.654000 | 1296.5000 | 1922.8600 |
| ORAL | 250 | 12.00 | 268.334000 | 855.5100 | 1432.2400 |
| ORAL | 250 | 16.00 | 113.282000 | 466.3600 | 970.7700 |
| ORAL | 250 | 24.00 | 11.168400 | 144.8100 | 558.9920 |

### BONUS: visualize the concentration time data with the quantiles underlaid

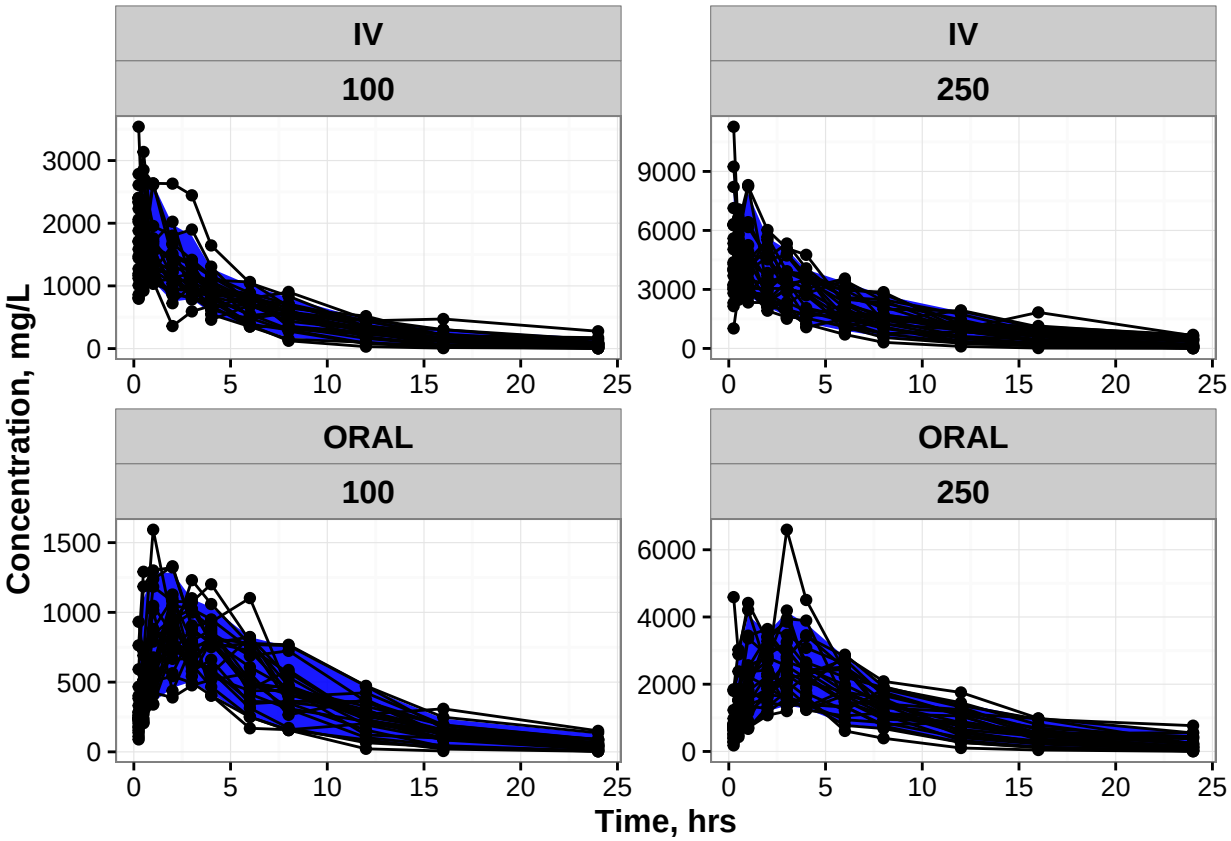
```
gg_form_dose <- pkdemog_cleaned %>%
  filter(!is.na(COBS)) %>%
  ggplot(aes(x = TIME, y = COBS, group = interaction(ID, FORM))) +
  geom_ribbon(data = quantile_summaries,
              aes(ymin = q05,
                  ymax = q95,
                  ## since don't have a y and group in this dataset but ggplot
                  ## will look since they are set in the base layer, need to set
                  ## them to null
                  y = NULL,
                  group = NULL),
              alpha = 0.9, fill = "blue") +
```

```
  geom_line() +
  geom_point()
```

```
gg_form_dose +
  facet_wrap(FORM~DOSE)
```




```
gg_form_dose +
  facet_wrap(FORM~DOSE, scales = "free") +
  theme_bw() +
  base_theme() +
  labs(
    x = "Time, hrs",
    y = "Concentration, mg/L"
  )
```


IV
100
IV
250
ORAL
100
ORAL
250
Concentration, mg/L
Time, hrs
0
1000
2000
3000
500
1500
3000
6000
9000
4000
0
5
10
15
20
25