Strawberries: exploratory data analysis

Jiaxin Li(U77902942)

2023-10-23

Jiaxin's EDA for strawberry data

Initial questions:

Initial questions about strawberries, the data, and about the work: The questions:

(1) What is the degree of harmfulness of each chemical, which chemicals are more harmful and which are relatively harmless?

(2) How are strawberries sold in different states and in different years? What about the use of chemicals?

(3) Whether there is a correlation between different variables, e.g., whether strawberry sales are related to the year or the state in which they are located, etc.

References

Here are references that helps me while I'm writing.

(Besides, thanks for Aidan's help about understanding variables, dealing with missing values, etc.)

NASS help

Quick Stats Glossary

Quick Stats Column Definitions

stats by subject

for EPA number lookup epa numbers

Active Pesticide Product Registration Informational Listing pc number input pesticide chemical search

toxic chemical dashboard

ACToR – Aggregated Computational Toxicology Resource

comptox dashboard

pubChem

Investigating toxic pesticides

References that are helpful here:

start here with chem PC code

step 2 to get label (with warnings) for products using the chemical

International Chemical safety cards

Pesticide Product and Label System

Search by Chemical

CompTox Chemicals Dashboard

Active Pesticide Product Registration Informational Listing

OSHA chemical database

Pesticide Ingredients

NPIC Product Research Online (NPRO)

Databases for Chemical Information

Pesticide Active Ingredients

TSCA Chemical Substance Inventory

glyphosate

Matching processes

First, I need to match different chemicals' PC codes, CAS numbers and their harm ranks.

To be more specific,

(1) The numbers following the equals sign in these chemical substance records typically represent CAS numbers (Chemical Abstracts Service Registry Numbers). CAS numbers are a standardized numbering system used to uniquely identify chemical substances. Each CAS number is unique and serves the purpose of ensuring accurate identification and retrieval of information about a specific chemical substance. These numbers do not typically convey direct toxicity or hazard meanings; instead, they are used for the unique identification of chemicals in scientific and legal documents;

(2) In the list of 171 chemical substance records, there are 89 unique CAS numbers. The reason there are not 171 unique CAS numbers is that some chemicals share the same CAS number. This can happen when multiple substances have similar chemical structures or active ingredients and are therefore assigned the same CAS number. CAS numbers are meant to uniquely identify chemical substances, but similar or equivalent substances may share the same CAS number in some cases.

Then, In order to match the subsequent PC codes with their corresponding CAS numbers, all the PC numbers in the "Data Items" column are first extracted into a new separate column variable using regular expressions.

```r
library(dplyr)
library(writexl)

strwb_survey_chem_CAS <- strwb_survey_chem |>
  mutate(chemical_name = sub(".*\\((.*?)\\s=.*", "\\1", temp43),
         PCcodes = sub(".*=\\s(.*?)\\)", "\\1", temp43)) |>
  select(Year, State, temp23, chemical_name, PCcodes, Value)

# colnames(strwb_survey_chem_CAS)
# View(strwb_survey_chem_CAS)
# write_xlsx(strwb_survey_chem_CAS, path = "strwb_survey_chem_CAS.xlsx")
```

Data visualization about the usage of the four main groups of chemicals

Data visualization was used here to initially explore the use of the four main groups of chemicals("FUNGICIDE", "HERBICIDE", "INSECTICIDE","OTHER") in different states in different years:

(1) Here I created line plots using ggplot2 to visualize the proportion of different chemicals usage over time (from 2016 to 2018 to 2019 to 2021) for four different states (CALIFORNIA, FLORIDA, OREGON, WASHINGTON). The proportion is defined as the count of a specific kind of chemical divided by the sum of the counts of the four types of chemicals: 'FUNGICIDE', 'HERBICIDE', 'INSECTICIDE' and 'OTHER';

(2) 'OREGON' and 'WASHINGTON' have data for 2016 but not for other years, it is likely due to a lack of data availability for these states in the subsequent years (2018, 2019, and 2021) in the data set. In other words, the data set we are working with might not include information for those states in those specific years, resulting in no data points for those combinations."

```
unique(strwb_survey_chem_CAS$Year)
```

```
[1] 2021 2019 2018 2016
```

```
unique(strwb_survey_chem_CAS$State)
```

```
[1] "CALIFORNIA" "FLORIDA"    "OREGON"     "WASHINGTON"
```

```
unique(strwb_survey_chem_CAS$temp23)
```

```
[1] " FUNGICIDE"   " HERBICIDE"   " INSECTICIDE" " OTHER"
```

```
library(ggplot2)
library(dplyr)

states_of_interest <- c("CALIFORNIA", "FLORIDA", "OREGON", "WASHINGTON")
filtered_data <- strwb_survey_chem_CAS %>%
  filter(State %in% states_of_interest)

proportion_data <- filtered_data %>%
  group_by(Year, State) %>%
  summarise(
    fungicide_count = sum(temp23 == " FUNGICIDE"),
    total_count = sum(temp23 %in% c(" FUNGICIDE", " HERBICIDE", " INSECTICIDE", " OTHER"))
  ) %>%
  mutate(proportion = round(fungicide_count / total_count, 3))
```

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

```
library(ggplot2)
library(dplyr)
library(gridExtra)
```

```

 'gridExtra'
```

```
The following object is masked from 'package:dplyr':

    combine
```

```
states_of_interest <- c("CALIFORNIA", "FLORIDA", "OREGON", "WASHINGTON")

create_lineplot <- function(temp23_label, title) {
  filtered_data <- strwb_survey_chem_CAS %>%
    filter(State %in% states_of_interest)

  proportion_data <- filtered_data %>%
    group_by(Year, State) %>%
    summarise(
      count = sum(temp23 == temp23_label),
      total_count = sum(temp23 %in% c(" FUNGICIDE", " HERBICIDE", " INSECTICIDE", " OTHER"
    ) %>%
    mutate(proportion = round(count / total_count, 3))

  lineplot <- ggplot(proportion_data, aes(x = Year, y = proportion, color = State)) +
    geom_line() +
    geom_point(aes(label = sprintf("%.3f", proportion)), size = 3) +
    labs(
      x = "Year",
      y = "Proportion",
      title = title
    ) +
    theme_minimal() +
    theme(legend.position = "top") + # Move the legend to the top
    guides(color = guide_legend(ncol = 2)) # Adjust the legend to have 2 columns
  return(lineplot)
}

lineplot1 <- create_lineplot(" FUNGICIDE", "The Proportion of the Utility of FUNGICIDE")
```

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

```
Warning in geom_point(aes(label = sprintf("%.3f", proportion)), size = 3):
Ignoring unknown aesthetics: label
```

```
lineplot2 <- create_lineplot(" HERBICIDE", "The Proportion of the Utility of HERBICIDE")
```

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

```
Warning in geom_point(aes(label = sprintf("%.3f", proportion)), size = 3):
Ignoring unknown aesthetics: label
```

```
lineplot3 <- create_lineplot(" INSECTICIDE", "The Proportion of the Utility of INSECTICIDE
```

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

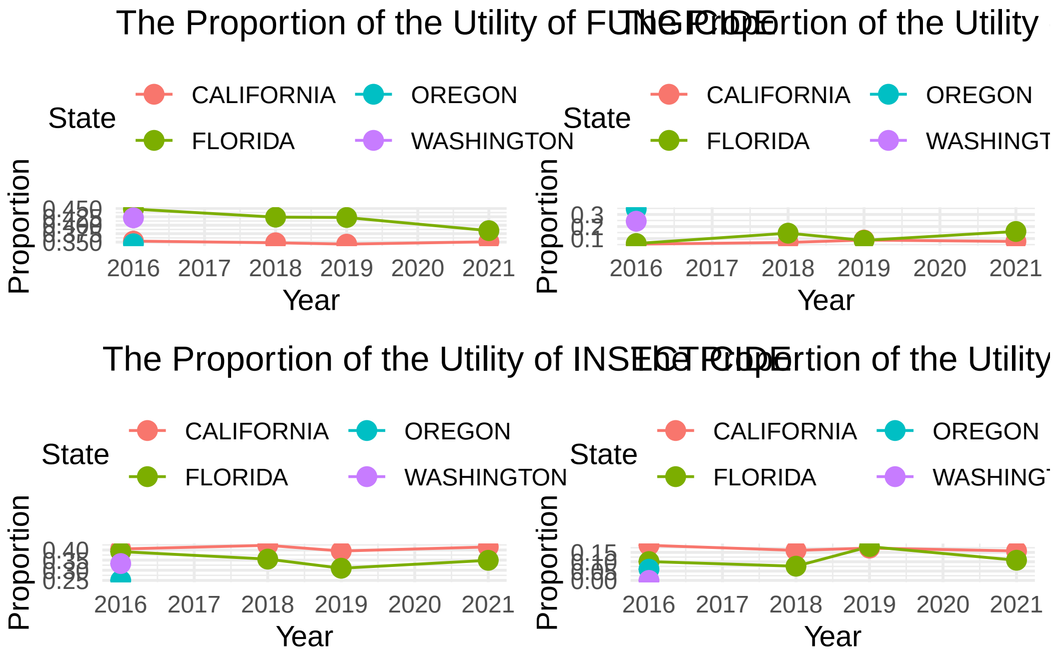
```
Warning in geom_point(aes(label = sprintf("%.3f", proportion)), size = 3):
Ignoring unknown aesthetics: label
```

```
lineplot4 <- create_lineplot(" OTHER", "The Proportion of the Utility of OTHER")
```

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

```
Warning in geom_point(aes(label = sprintf("%.3f", proportion)), size = 3):
Ignoring unknown aesthetics: label
```

```r
grid.arrange(lineplot1, lineplot2, lineplot3, lineplot4, ncol = 2)
```



Here, we could quickly check that there is data missing, definitely. And take the 2018 year for an example:

```r
desired_year <- 2018
desired_state <- "OREGON"

subset_data <- subset(strwb_survey_chem_CAS, Year == desired_year & State == desired_state
print(subset_data)
```

```
# A tibble: 0 x 6
# i 6 variables: Year <dbl>, State <chr>, temp23 <chr>, chemical_name <chr>,
#   PCcodes <chr>, Value <chr>
```

```r
desired_year <- 2018
desired_state <- "WASHINGTON"

subset_data <- subset(strwb_survey_chem_CAS, Year == desired_year & State == desired_state
# print(subset_data)
```

```
strwb_survey_mkt <- strwb_survey_mkt[!grepl("\\(D\\)", strwb_survey_mkt$Value), ]
strwb_survey_mkt$Value <- as.numeric(strwb_survey_mkt$Value)
```

```
Warning:       NA
```

```
strwb_survey_mkt_grouped <- strwb_survey_mkt |>
  group_by(Year, State, temp1b) |>
  summarise(
    average_value = mean(Value)
  )
```

```
`summarise()` has grouped output by 'Year', 'State'. You can override using the
`.groups` argument.
```

```
# View(strwb_survey_mkt_grouped)
```

Exploring different chemicals' harm ranks

In the following, I will match the PC codes of the chemical substances in the existing dataset to their corresponding CAS numbers, and then match them to the hazard classes of the corresponding chemical substances, with the help of the EXCEL datasheet provided by the professor, which contains CAS numbers and hazard classes.

And about the harms of different chemicals with different CAS numbers, we can learn from the file that prof shared that "INDEX. CLASS IFICATION OF PESTICIDE AC TIVE INGREDIENTS: Ia = Extremely hazardous; Ib= Highly hazardous; II=Moderately hazardous; III=Slightly hazardous; U = Unlikely to present acute hazard in normal use; FM =Fumigant, not classified; O = Obsolete as pesticide, not classified."

```
cas_and_harm <- readxl::read_xlsx("CAS.xlsx")
# View(cas_and_harm)
```

```
cas <- as.vector(unique(strwb_survey_chem_CAS$PCcodes))

PCcodes <- cas[nchar(cas) == 6 & grepl("^[0-9]+$", cas)]
PCcodes <- as.data.frame(PCcodes)
PCcodes$cas_valid <- c("23564-05-8", "15299-99-7", "38641-94-0", "70901-12-1", "13356-08-6
# View(PCcodes)
```

```
library(dplyr)
strwb_survey_chem_CAS <- merge(strwb_survey_chem_CAS, PCcodes, by = "PCcodes")
strwb_survey_chem_CAS <- merge(strwb_survey_chem_CAS, cas_and_harm, by = "cas_valid")
# View(strwb_survey_chem_CAS)
# write_xlsx(strwb_survey_chem_CAS, path = "data_ with_cas_and_harms.xlsx")
```

Dealing with the missing values

Handling of missing values in the "Value" variable: Calculate the mean value of the "Value" variable from valid values other than "(D)" and assign this calculated mean value to "(D)", "(NA)" and "(Z)". (Thanks for Aidan's inspiration here!)

```
non_numeric_values <- c("(D)", "(NA)", "(Z)")
strwb_survey_chem_CAS$Value[strwb_survey_chem_CAS$Value %in% non_numeric_values] <- NA
mean_value <- mean(as.numeric(strwb_survey_chem_CAS$Value), na.rm = TRUE)
```

```
Warning in mean(as.numeric(strwb_survey_chem_CAS$Value), na.rm = TRUE):
     NA
```

```
strwb_survey_chem_CAS$Value[is.na(strwb_survey_chem_CAS$Value)] <- mean_value
strwb_survey_chem_CAS$Value <- as.numeric(strwb_survey_chem_CAS$Value)
```

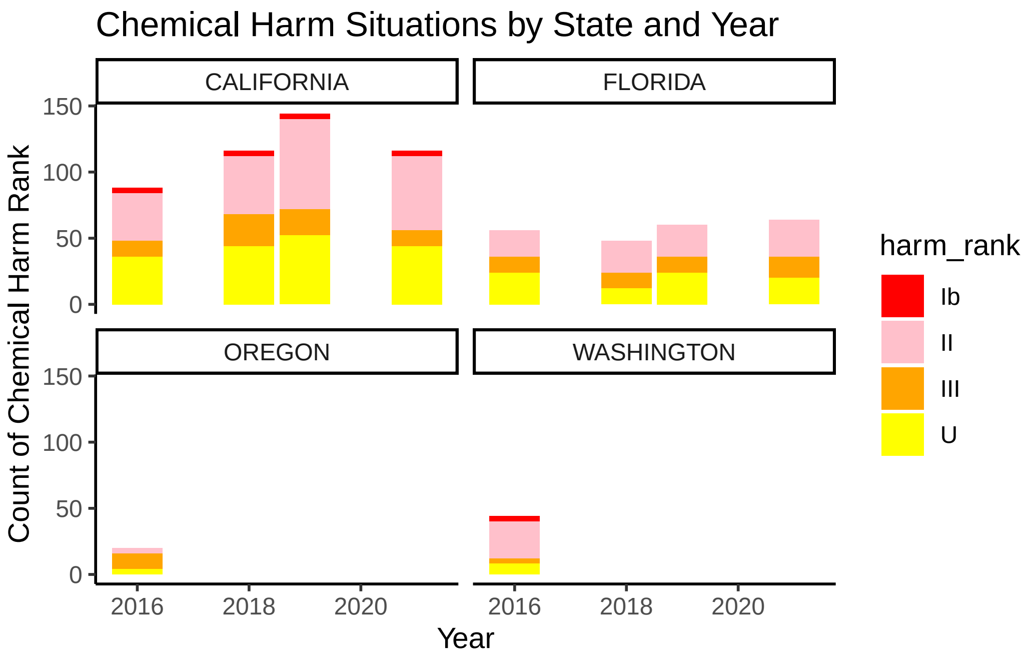
```
Warning:      NA
```

```
strwb_survey_chem_CAS$Value <-round(strwb_survey_chem_CAS$Value, digits = 3)

head(strwb_survey_chem_CAS)
```

```
    cas_valid PCcodes Year   State     temp23 chemical_name  Value harm_rank
1 103361-09-7  121011 2021 FLORIDA  HERBICIDE     CLETHODIM 38.188       III
2 103361-09-7  121011 2016  OREGON  HERBICIDE     CLETHODIM 38.188       III
3 103361-09-7  121011 2016  OREGON  HERBICIDE     CLETHODIM 38.188       III
4 103361-09-7  121011 2021 FLORIDA  HERBICIDE     CLETHODIM 38.188       III
5 103361-09-7  121011 2021 FLORIDA  HERBICIDE     CLETHODIM 38.188       III
6 103361-09-7  121011 2016  OREGON  HERBICIDE     CLETHODIM 38.188       III
```

```
#colnames(strwb_survey_chem_CAS)
#unique(strwb_survey_chem_CAS$harm_rank)
#unique(strwb_survey_chem_CAS$Year)
#unique(strwb_survey_chem_CAS$State)
```

```
library(ggplot2)
ggplot(data = strwb_survey_chem_CAS, aes(x = Year, fill = harm_rank)) +
  geom_bar(position = "stack") +
  facet_wrap(~ State) +
  labs(title = "Chemical Harm Situations by State and Year",
       x = "Year",
       y = "Count of Chemical Harm Rank") +
  scale_fill_manual(values = c("Ib" = "red", "II" = "pink", "III" = "orange", "U" = "yello
  theme_classic()
```



From this, it can be seen that the harm ranks of chemicals used in different states in different years are predominantly II(Moderately hazardous) and U(Unlikely to present acute hazard in normal use.) different years is predominantly level 2 and level 5, which means that the hazards of the chemicals used between 2016 and 2021 are relatively acceptable.

Data distributions and regression models

exploring different states' situations about the harm ranks of chemicals

In addition, although the above analysis of the hazards of chemical substances has been carried out on a granular basis for each chemical substance, there are other factors that may have an impact on the harmlessness of different chemical substances in practice, such as the dosage used, whether strawberries are washed carefully, and so on.

explore data in data frame "strwb_survey_chem" and "strwb_survey_mkt"

Here I want to explore data in data frame "strwb_survey_chem", especially I'm curious about the relationships among variables like "State", "Year", "Value". So I deal with the missing values in column "Value" first, then I could try to create some visualization plots and fit some models as below. This means that

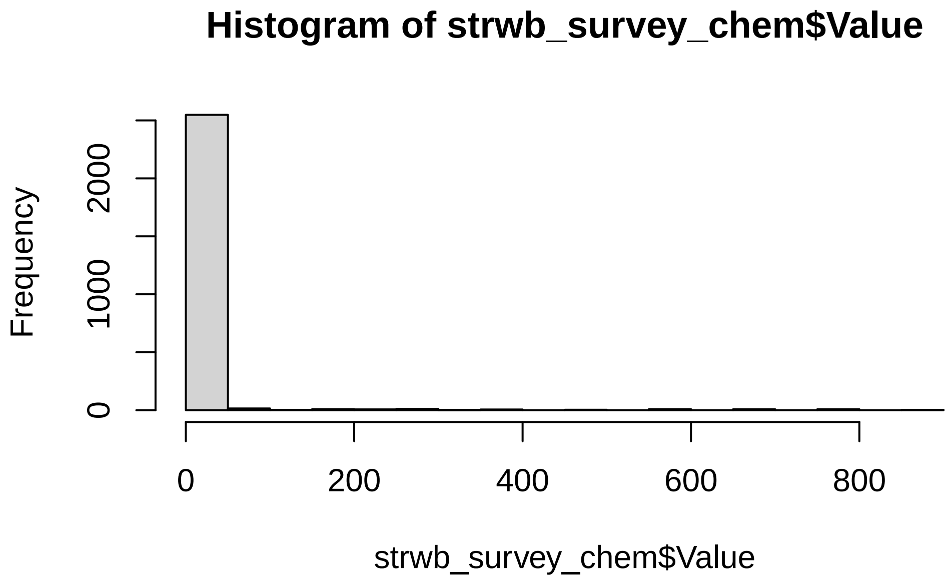
```
non_numeric_values <- c("(D)", "(NA)", "(Z)")
strwb_survey_chem$Value[strwb_survey_chem$Value %in% non_numeric_values] <- NA
mean_value <- mean(as.numeric(strwb_survey_chem$Value), na.rm = TRUE)
```

```
Warning in mean(as.numeric(strwb_survey_chem$Value), na.rm = TRUE):
     NA
```

```
strwb_survey_chem$Value[is.na(strwb_survey_chem$Value)] <- mean_value
strwb_survey_chem$Value <- as.numeric(strwb_survey_chem$Value)
```

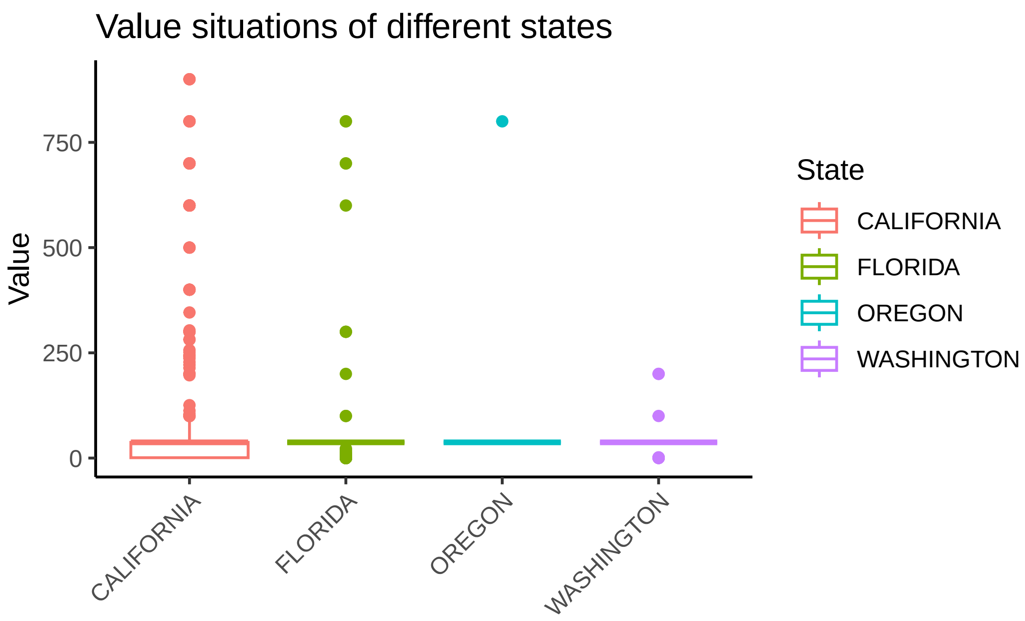
```
Warning:       NA
```

```
strwb_survey_chem$Value <-round(strwb_survey_chem$Value, digits = 3)
# View(strwb_survey_chem)

hist(strwb_survey_chem$Value)
```



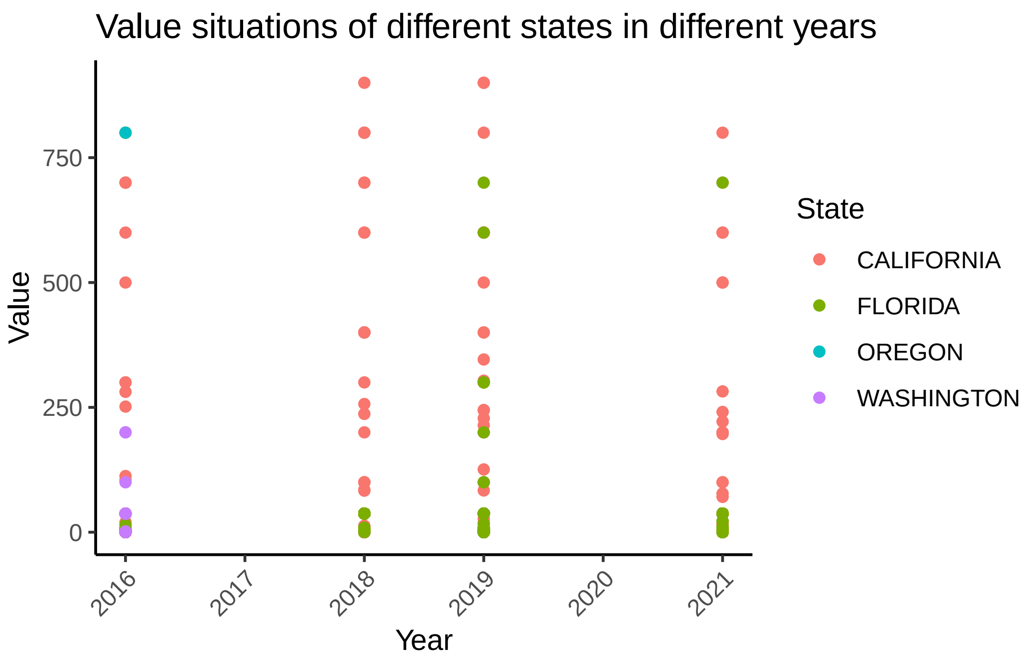
```
ggplot(data = strwb_survey_chem, aes(x=State, y=Value, color = State)) +
  geom_boxplot() +
  theme_classic() +
  theme(axis.text.x = element_text(angle = 45, vjust = 1, hjust = 1)) +
  labs(
    title = "Value situations of different states"
  )
```

```
Warning: Removed 246 rows containing non-finite values (`stat_boxplot()`).
```



```
ggplot(data = strwb_survey_chem, aes(x=Year, y=Value, color = State)) +
  geom_point() +
  theme_classic() +
  theme(axis.text.x = element_text(angle = 45, vjust = 1, hjust = 1)) +
  labs(
    title = "Value situations of different states in different years"
  )
```

```
Warning: Removed 246 rows containing missing values (`geom_point()`).
```



Then I try to explore whether the factors like state, year, chemical types could influence the Value, so I fit a generalized linear model(model1) and linear model(model2) below.

But in both outputs, many coefficients has relatively large standard deviation, and the t-stat indicates I fail to reject the Null Hypothesis(All the coefficients are equal to zero), so these two model don't perform well. In the future, I will try more model to explore which model could fit well.

It turns out that the variable data are over dispersed so there are many outliers and the usual linear models don't perform well.

```
library(rstanarm)
```

```
    Rcpp

This is rstanarm version 2.21.4

- See https://mc-stan.org/rstanarm/articles/priors for changes to default priors!

- Default priors may change, so it's safest to specify priors, even if equivalent to the defa

- For execution on a local, multicore CPU with excess RAM we recommend calling
```

```
options(mc.cores = parallel::detectCores())
```

```
model1 <- stan_glm(Value~Year + State + temp23, data=strwb_survey_chem, refresh=0)
summary(model1)
```

```
Model Info:
 function:     stan_glm
 family:       gaussian [identity]
 formula:      Value ~ Year + State + temp23
 algorithm:    sampling
 sample:       4000 (posterior sample size)
 priors:       see help('prior_summary')
 observations: 2633
 predictors:   8

Estimates:
                     mean    sd      10%     50%     90%
(Intercept)          221.5  1840.4 -2113.5   202.1  2630.6
Year                  -0.1     0.9    -1.3    -0.1     1.1
StateFLORIDA           3.0     3.4    -1.3     2.9     7.3
StateOREGON           11.2     9.6    -1.0    10.9    23.7
StateWASHINGTON        3.4     7.7    -6.3     3.3    13.2
temp23 HERBICIDE       8.6     5.6     1.5     8.6    15.7
temp23 INSECTICIDE    10.9     3.6     6.2    11.0    15.6
temp23 OTHER          15.4     5.1     8.9    15.4    21.9
sigma                 81.3     1.1    79.8    81.2    82.7

Fit Diagnostics:
           mean   sd   10%   50%   90%
mean_PPD 37.3    2.2 34.5  37.3  40.2

The mean_ppd is the sample average posterior predictive distribution of the outcome variable

MCMC diagnostics
                   mcse Rhat n_eff
(Intercept)        28.0  1.0 4330
Year                0.0  1.0 4331
StateFLORIDA        0.1  1.0 4248
StateOREGON         0.1  1.0 4185
StateWASHINGTON     0.1  1.0 3981
```

```
temp23 HERBICIDE    0.1  1.0 4991
temp23 INSECTICIDE  0.1  1.0 4276
temp23 OTHER        0.1  1.0 4158
sigma               0.0  1.0 4271
mean_PPD            0.0  1.0 4302
log-posterior       0.1  1.0 1644

For each parameter, mcse is Monte Carlo standard error, n_eff is a crude measure of effectiv
```

```
model2 <- lm(Value~Year + State + temp23, data=strwb_survey_chem)
summary(model2)
```

```

Call:
lm(formula = Value ~ Year + State + temp23, data = strwb_survey_chem)

Residuals:
   Min     1Q Median     3Q    Max 
-43.97 -27.76  -5.31   0.34 871.60 

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)   
(Intercept)         280.8700  1849.5516   0.152  0.87931   
Year                 -0.1250     0.9163  -0.136  0.89146   
StateFLORIDA          2.9301     3.4411   0.852  0.39456   
StateOREGON          11.0538     9.6052   1.151  0.24991   
StateWASHINGTON       3.2225     7.8243   0.412  0.68047   
temp23 HERBICIDE      8.5870     5.6532   1.519  0.12889   
temp23 INSECTICIDE   10.9387     3.6665   2.983  0.00288 **
temp23 OTHER         15.3162     4.9430   3.099  0.00197 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 81.24 on 2625 degrees of freedom
  (   246    )
Multiple R-squared:  0.005629,  Adjusted R-squared:  0.002977 
F-statistic: 2.123 on 7 and 2625 DF,  p-value: 0.03821
```

The last part of my EDA is about exploring data in the "strwb_survey_mkt", to explore the relationships among "state", "year", "Value", etc.

```r
mean_value <- mean(as.numeric(strwb_survey_mkt$Value), na.rm = TRUE)
strwb_survey_mkt$Value[is.na(strwb_survey_mkt$Value)] <- mean_value
strwb_survey_mkt$Value <-round(strwb_survey_mkt$Value, digits = 3)
# View(strwb_survey_mkt)


model3 <- stan_glm(Value~Year + State, data=strwb_survey_mkt, refresh=0)
summary(model1)
```

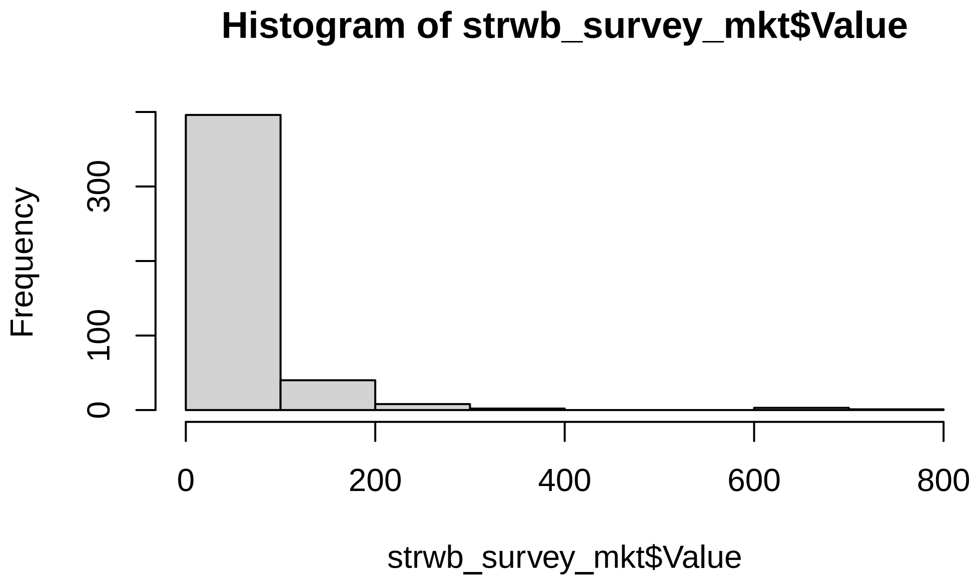
```
Model Info:
 function:     stan_glm
 family:       gaussian [identity]
 formula:      Value ~ Year + State + temp23
 algorithm:    sampling
 sample:       4000 (posterior sample size)
 priors:       see help('prior_summary')
 observations: 2633
 predictors:   8

Estimates:
                     mean   sd     10%    50%    90%
(Intercept)         221.5 1840.4 -2113.5  202.1 2630.6
Year                 -0.1    0.9    -1.3   -0.1    1.1
StateFLORIDA          3.0    3.4    -1.3    2.9    7.3
StateOREGON          11.2    9.6    -1.0   10.9   23.7
StateWASHINGTON       3.4    7.7    -6.3    3.3   13.2
temp23 HERBICIDE      8.6    5.6     1.5    8.6   15.7
temp23 INSECTICIDE   10.9    3.6     6.2   11.0   15.6
temp23 OTHER         15.4    5.1     8.9   15.4   21.9
sigma                81.3    1.1    79.8   81.2   82.7

Fit Diagnostics:
           mean   sd   10%   50%   90%
mean_PPD 37.3    2.2 34.5  37.3  40.2

The mean_ppd is the sample average posterior predictive distribution of the outcome variable

MCMC diagnostics
                   mcse Rhat n_eff
(Intercept)        28.0  1.0 4330
Year                0.0  1.0 4331
```

```
StateFLORIDA        0.1  1.0 4248
StateOREGON         0.1  1.0 4185
StateWASHINGTON     0.1  1.0 3981
temp23 HERBICIDE    0.1  1.0 4991
temp23 INSECTICIDE  0.1  1.0 4276
temp23 OTHER        0.1  1.0 4158
sigma               0.0  1.0 4271
mean_PPD            0.0  1.0 4302
log-posterior       0.1  1.0 1644

For each parameter, mcse is Monte Carlo standard error, n_eff is a crude measure of effective
```

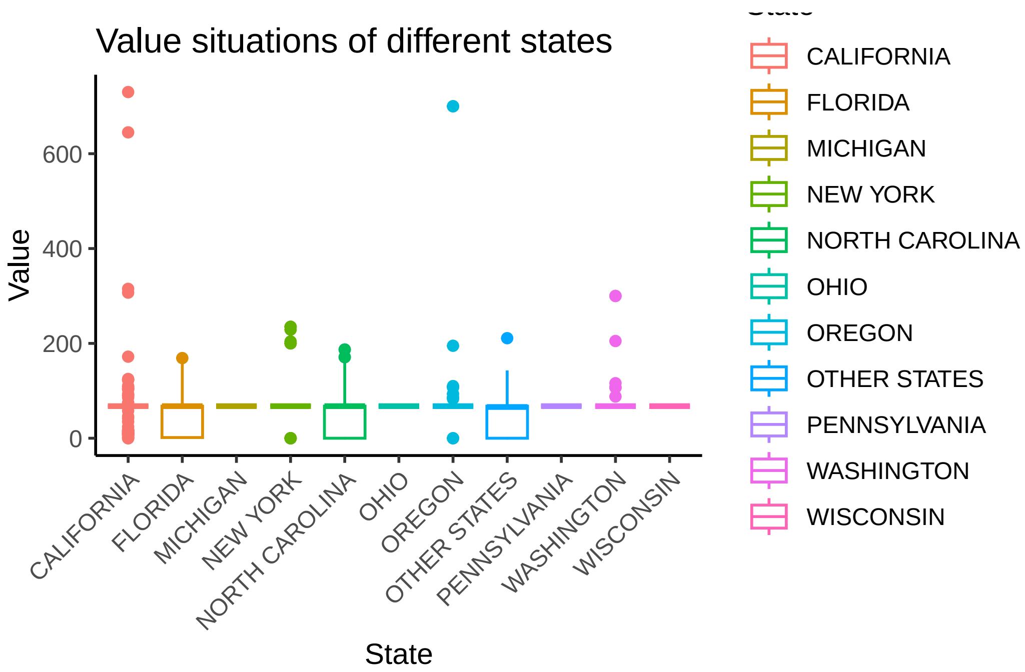
```
model4 <- lm(Value~Year + State, data=strwb_survey_mkt)
summary(model2)
```

```

Call:
lm(formula = Value ~ Year + State + temp23, data = strwb_survey_chem)

Residuals:
   Min     1Q Median     3Q    Max 
-43.97 -27.76  -5.31   0.34 871.60 

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)   
(Intercept)         280.8700  1849.5516   0.152  0.87931   
Year                 -0.1250     0.9163  -0.136  0.89146   
StateFLORIDA          2.9301     3.4411   0.852  0.39456   
StateOREGON          11.0538     9.6052   1.151  0.24991   
StateWASHINGTON       3.2225     7.8243   0.412  0.68047   
temp23 HERBICIDE      8.5870     5.6532   1.519  0.12889   
temp23 INSECTICIDE   10.9387     3.6665   2.983  0.00288 **
temp23 OTHER         15.3162     4.9430   3.099  0.00197 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 81.24 on 2625 degrees of freedom
  (   246    )
Multiple R-squared:  0.005629,  Adjusted R-squared:  0.002977 
F-statistic: 2.123 on 7 and 2625 DF,  p-value: 0.03821
```

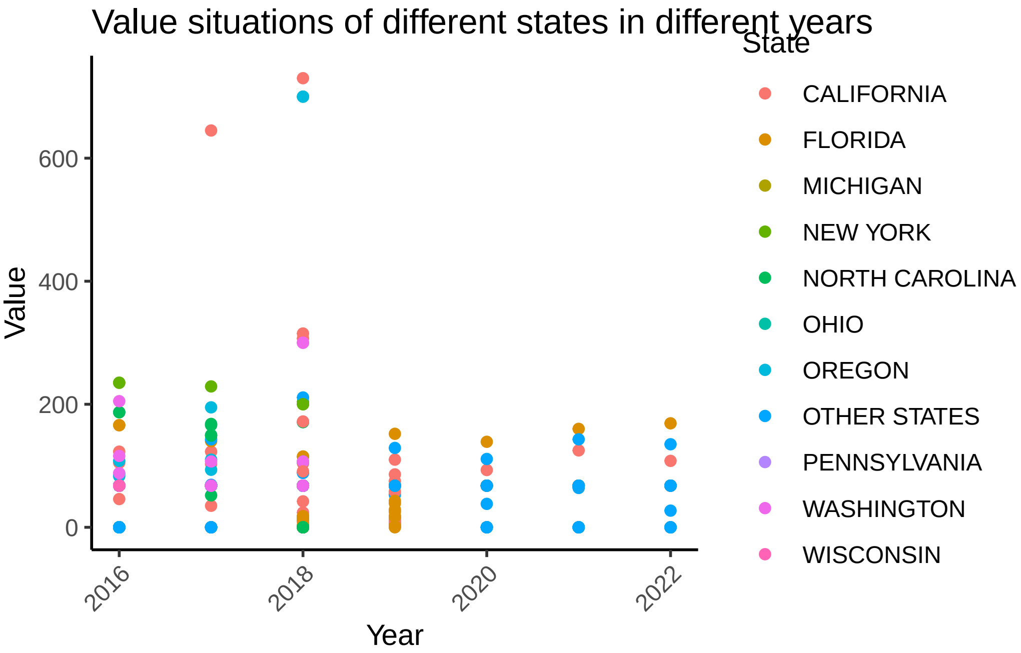
```
hist(strwb_survey_mkt$Value)
```



```
ggplot(data = strwb_survey_mkt, aes(x=State, y=Value, color = State)) +
  geom_boxplot() +
  theme_classic() +
  theme(axis.text.x = element_text(angle = 45, vjust = 1, hjust = 1)) +
  labs(
    title = "Value situations of different states"
  )
```



```
ggplot(data = strwb_survey_mkt, aes(x=Year, y=Value, color = State)) +
  geom_point() +
  theme_classic() +
  theme(axis.text.x = element_text(angle = 45, vjust = 1, hjust = 1)) +
  labs(
    title = "Value situations of different states in different years"
  )
```


Value situations of different states in different years
Value
600
400
200
0
Year
2016
2018
2020
2022
State
CALIFORNIA
FLORIDA
MICHIGAN
NEW YORK
NORTH CAROLINA
OHIO
OREGON
OTHER STATES
PENNSYLVANIA
WASHINGTON
WISCONSIN