Stawberries: exploratory data analysis

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Jiaxin's EDA for strawberry data

These references have been left in the document to help while you are writing. Cite those you use and drop the rest from the final document.

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

The EPA PC (Pesticide Chemical) Code is a unique chemical code number assigned by the EPA to a particular pesticide active ingredient, inert ingredient or mixture of active ingredients.

Investigating toxic pesticides

```
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
То
  # View(strwb_census)
  # View(strwb_survey)
  # View(strwb_survey_mkt)
  # View(strwb_survey_chem)
  unique(strwb_survey_mkt$temp1b)
[1] "PRICE RECEIVED" NA
                                          "PRODUCTION"
  unique(strwb_survey_mkt$temp2)
```

```
[1] " MEASURED IN $ / CWT"
                                      " FRESH MARKET - PRICE RECEIVED"
 [3] " PROCESSING - PRICE RECEIVED" " MEASURED IN $"
 [5] " MEASURED IN CWT"
                                      " FRESH MARKET - PRODUCTION"
 [7] " FRESH MARKET"
                                      " NOT SOLD - PRODUCTION"
 [9] " PROCESSING - PRODUCTION"
                                     " PROCESSING"
[11] " UTILIZED - PRODUCTION"
                                     " MEASURED IN TONS"
[13] " BEARING - APPLICATIONS"
  unique(strwb_survey_mkt$temp3)
 [1] NA
 [2] " MEASURED IN $ / CWT"
 [3] " MEASURED IN $"
 [4] " UTILIZED - PRODUCTION"
 [5] " MEASURED IN CWT"
 [6] " MEASURED IN TONS"
 [7] " MEASURED IN LB"
 [8] " MEASURED IN LB / ACRE / APPLICATION"
 [9] " MEASURED IN LB / ACRE / YEAR"
[10] " MEASURED IN NUMBER"
[11] " MEASURED IN $ / TON"
  unique(strwb_survey_mkt$temp4)
                        " MEASURED IN CWT" " AVG"
[1] NA
[4] " MEASURED IN TONS"
 unique(strwb_survey_mkt$temp42)
[1] "NOT SPECIFIED"
                             "FERTILIZER: (NITROGEN)"
[3] "FERTILIZER: (PHOSPHATE)" "FERTILIZER: (POTASH)"
[5] "FERTILIZER: (SULFUR)"
  unique(strwb_survey_chem$temp4)
[1] NA
           " AVG"
```

```
unique(strwb_survey_chem$temp23)
[1] " FUNGICIDE" " HERBICIDE" " INSECTICIDE" " OTHER"
# unique(strwb_survey_chem$temp43)
```

- (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.

[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"
```

Data visualisation 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."

```
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))
```

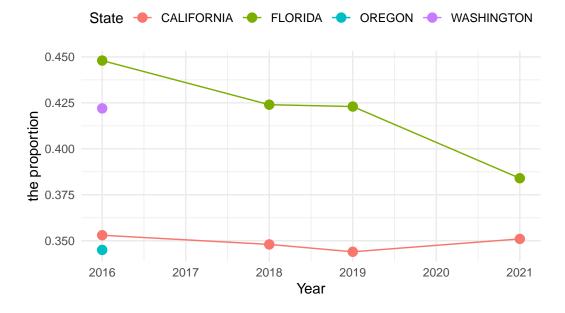
`summarise()` has grouped output by 'Year'. You can override using the `.groups` argument.

```
lineplot1 <- 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 = "the proportion",
        title = "The Proportion of the Utility of Fungicide"
    ) +
    theme_minimal() +
    theme(legend.position = "top")</pre>
```

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

lineplot1

The Proportion of the Utility of Fungicide



```
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 == " HERBICIDE"),
      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.
  lineplot2 <- ggplot(proportion_data, aes(x = Year, y = proportion, color = State)) +
    geom_line() +
    geom_point(aes(label = sprintf("%.3f", proportion)), size = 3) +
      x = "Year",
      y = "the proportion",
      title = "The Proportion of the Utility of HERBICIDE"
    ) +
    theme_minimal() +
    theme(legend.position = "top")
Warning in geom_point(aes(label = sprintf("%.3f", proportion)), size = 3):
Ignoring unknown aesthetics: label
```

The Proportion of the Utility of HERBICIDE



```
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 == " INSECTICIDE"),
    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.

lineplot3 <- ggplot(proportion_data, aes(x = Year, y = proportion, color = State)) +
  geom_line() +
  geom_point(aes(label = sprintf("%.3f", proportion)), size = 3) +
  labs(
    x = "Year",</pre>
```

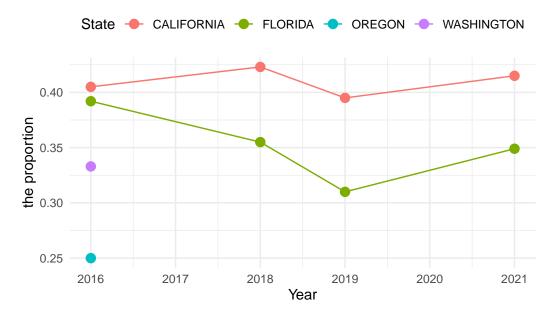
y = "the proportion",

```
title = "The Proportion of the Utility of INSECTICIDE"
) +
theme_minimal() +
theme(legend.position = "top")
```

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

lineplot3

The Proportion of the Utility of INSECTICIDE



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

# Calculate the count of "FUNGICIDE" and the total count of all chemical types for each coproportion_data <- filtered_data %>%
  group_by(Year, State) %>%
  summarise(
  fungicide_count = sum(temp23 == "OTHER"),
  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.
  lineplot4 <- 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 = "the proportion",
      title = "The Proportion of the Utility of OTHER"
    theme_minimal() +
    theme(legend.position = "top")
Warning in geom_point(aes(label = sprintf("%.3f", proportion)), size = 3):
Ignoring unknown aesthetics: label
  lineplot4
```

The Proportion of the Utility of OTHER



```
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>
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[!grep1("\\(D\\))", strwb_survey_mkt$Value), ]
strwb_survey_mkt$Value <- as.numeric(strwb_survey_mkt$Value)</pre>
```

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)
```

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)

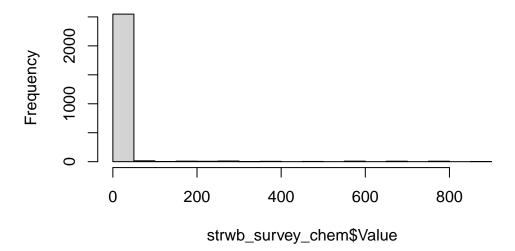
library(dplyr)
strwb_survey_chem_CAS <- merge(strwb_survey_chem_CAS, PCcodes, by = "PCcodes")
strwb_survey_chem_CAS <- merge(strwb_survey_chem_CAS, cas_and_harm, by = "cas_valid")
# View(strwb_survey_chem_CAS)
# write_xlsx(strwb_survey_chem_CAS, path = "data_ with_cas_and_harms.xlsx")</pre>
```

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!!! He's an angel and a genius!!!)

```
non_numeric_values <- c("(D)", "(NA)", "(Z)")</pre>
  strwb_survey_chem_CAS$Value[strwb_survey_chem_CAS$Value %in% non_numeric_values] <- NA
  mean_value <- mean(as.numeric(strwb_survey_chem_CAS$Value), na.rm = TRUE)</pre>
Warning in mean(as.numeric(strwb_survey_chem_CAS$Value), na.rm = TRUE):
  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)
[1] "cas_valid"
                    "PCcodes"
                                     "Year"
                                                     "State"
[5] "temp23"
                    "chemical_name" "Value"
                                                     "harm_rank"
  unique(strwb_survey_chem_CAS$harm_rank)
[1] "III" "II"
                      "Ib"
```

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.

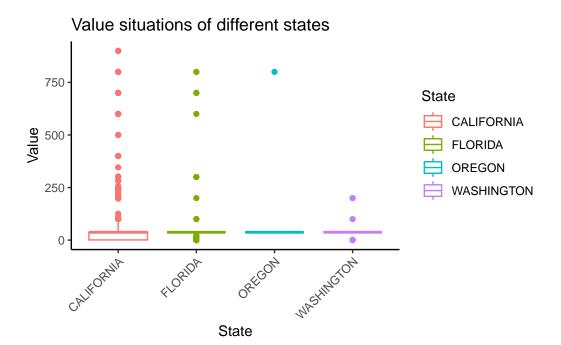
Histogram of strwb_survey_chem\$Value



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"
  )
```

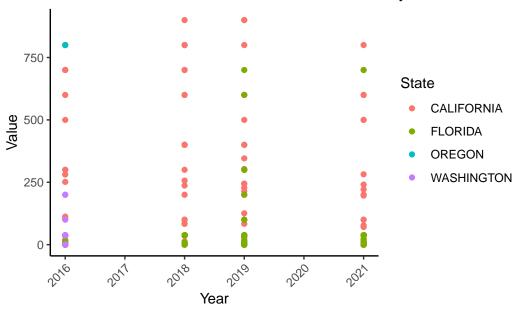
Warning: Removed 246 rows containing non-finite values (`stat_boxplot()`).



```
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 def
- 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)</pre>

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)	273.8	1863.9	-2097.4	278.3	2662.8
Year	-0.1	0.9	-1.3	-0.1	1.1
StateFLORIDA	3.0	3.4	-1.2	2.9	7.4
StateOREGON	11.0	9.8	-1.8	11.1	23.4
StateWASHINGTON	3.3	7.8	-6.7	3.4	13.3
temp23 HERBICIDE	8.5	5.8	1.0	8.5	15.9
temp23 INSECTICIDE	10.8	3.7	6.0	10.9	15.7
temp23 OTHER	15.3	4.9	8.9	15.3	21.5
sigma	81.3	1.1	79.8	81.3	82.6

Fit Diagnostics:

mean sd 10% 50% 90% mean_PPD 37.3 2.3 34.4 37.3 40.1

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

MCMC diagnostics

	mcse	Rhat	n_eff
(Intercept)	29.2	1.0	4080
Year	0.0	1.0	4081
StateFLORIDA	0.1	1.0	4300
StateOREGON	0.1	1.0	4604
StateWASHINGTON	0.1	1.0	3886

```
temp23 HERBICIDE0.11.04272temp23 INSECTICIDE0.11.03488temp23 OTHER0.11.03703sigma0.01.04491mean_PPD0.01.04045log-posterior0.11.01641
```

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

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

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	5 '.' 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.

```
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)</pre>
```

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)	273.8	1863.9	-2097.4	278.3	2662.8
Year	-0.1	0.9	-1.3	-0.1	1.1
StateFLORIDA	3.0	3.4	-1.2	2.9	7.4
StateOREGON	11.0	9.8	-1.8	11.1	23.4
StateWASHINGTON	3.3	7.8	-6.7	3.4	13.3
temp23 HERBICIDE	8.5	5.8	1.0	8.5	15.9
temp23 INSECTICIDE	10.8	3.7	6.0	10.9	15.7
temp23 OTHER	15.3	4.9	8.9	15.3	21.5
sigma	81.3	1.1	79.8	81.3	82.6

Fit Diagnostics:

mean sd 10% 50% 90% mean_PPD 37.3 2.3 34.4 37.3 40.1

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

MCMC diagnostics

```
StateFLORIDA
                  0.1 1.0 4300
StateOREGON
                  0.1 1.0 4604
StateWASHINGTON
                  0.1 1.0 3886
temp23 HERBICIDE
                  0.1 1.0 4272
temp23 INSECTICIDE 0.1 1.0 3488
temp23 OTHER
                  0.1 1.0 3703
sigma
                  0.0 1.0 4491
mean_PPD
                  0.0 1.0 4045
log-posterior
                  0.1 1.0 1641
```

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)</pre>
summary(model2)
```

Call:

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

Residuals:

1Q Median Min 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 **

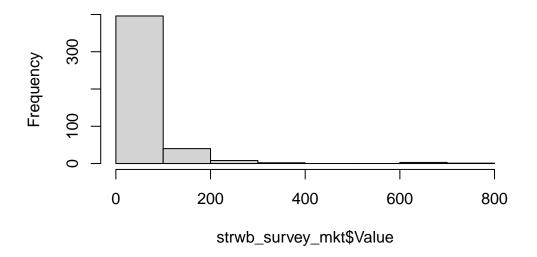
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 81.24 on 2625 degrees of freedom 246

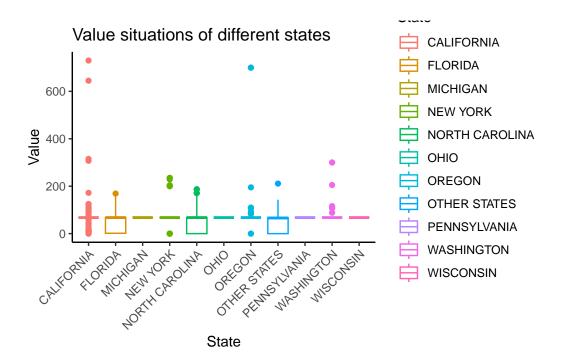
Multiple R-squared: 0.005629, Adjusted R-squared: 0.002977

F-statistic: 2.123 on 7 and 2625 DF, p-value: 0.03821

Histogram of 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"
)
```

