Monday, Mar 4

Proportions as Response Variables

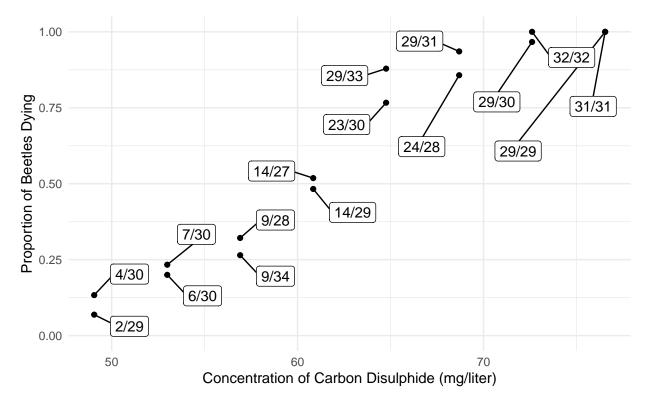
Consider the following data from an experiment that exposed batches of beetles to carbon disulphide.

```
library(trtools)
library(ggplot2)
library(ggrepel)

bliss$proportion <- paste(bliss$dead, "/", bliss$exposed, sep = "")
bliss</pre>
```

```
concentration dead exposed proportion
            49.06
1
                             29
                                       2/29
            49.06
2
                             30
                                       4/30
3
            52.99
                     7
                             30
                                       7/30
4
            52.99
                     6
                             30
                                       6/30
5
            56.91
                             28
                                       9/28
6
            56.91
                     9
                             34
                                       9/34
7
            60.84
                     14
                             27
                                      14/27
                             29
8
            60.84
                     14
                                      14/29
9
            64.76
                    23
                             30
                                      23/30
10
            64.76
                    29
                             33
                                      29/33
11
            68.69
                    29
                             31
                                      29/31
12
            68.69
                    24
                             28
                                      24/28
                                      29/30
13
            72.61
                    29
                             30
14
            72.61
                    32
                             32
                                      32/32
15
            76.54
                    29
                             29
                                      29/29
            76.54
                    31
                             31
                                      31/31
16
```

```
p <- ggplot(bliss, aes(x = concentration, y = dead/exposed)) +
  geom_point() + ylim(0, 1) + theme_minimal() +
  geom_label_repel(aes(label = proportion), box.padding = 0.75) +
  labs(x = "Concentration of Carbon Disulphide (mg/liter)",
      y = "Proportion of Beetles Dying")
plot(p)</pre>
```



The interest here is in modeling the *proportion* of dead beetles as a response variable.

A proportion Y_i can be defined as $Y_i = C_i/m_i$ where C_i is a count and m_i is a total so that $C_i = 0, 1, ..., m_i$ and $Y_i = 0, 1/m_i, 2/m_i, ..., 1$. Note that proportions are not quite the same as rates. Proportions are bounded between zero and one, but rates are only bounded below by zero.

- 1. Proportions may require nonlinear models because $0 \le E(Y_i) \le 1$.
- 2. Proportions tend to exhibit heteroscedasticty with variance depending on $E(Y_i)$ and m_i . The variance of Y_i tends to be smaller as $E(Y_i)$ gets closer to zero or one, and is inversely proportional to m_i .
- 3. Non-normal discrete distribution.

The Binomial Distribution

Assume m independent "trials" with a probability of a "success" on each trial of p (and thus the probability of a "failure" is 1-p). The number of successes then has a binomial distribution such that

$$P(C=c) = \binom{m}{c} p^c (1-p)^{m-c}$$

where

$$\binom{m}{c} = \frac{m!}{c!(m-c)!}.$$

The possible values of C are $0, 1, \ldots, m$. Note that $\binom{m}{c}$ is the number of outcomes where we can have a count of c out of m, and $p^c(1-p)^{m-c}$ is the probability of each of these outcomes.

Example: Suppose that the probability of observing a seed germinate under certain conditions is 0.2, and we observe four seeds. Let C be the number of seeds that germinate. Then m = 4 and p = 0.2. The probability that, say, C = 3 is then

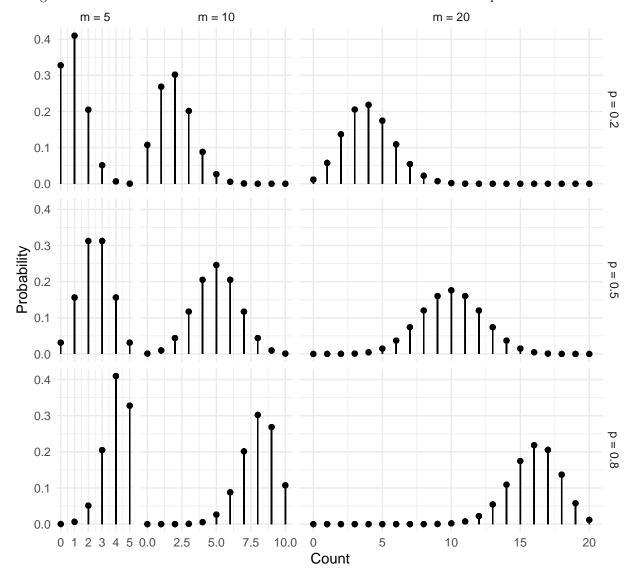
$$P(C=3) = \underbrace{\frac{4!}{3!(4-3)!}}_{4} \underbrace{0.2^{3}(1-0.2)^{4-3}}_{0.0064} = 0.0246.$$

There are four outcomes that give three successes, and each of these outcomes has a probability of 0.0064.

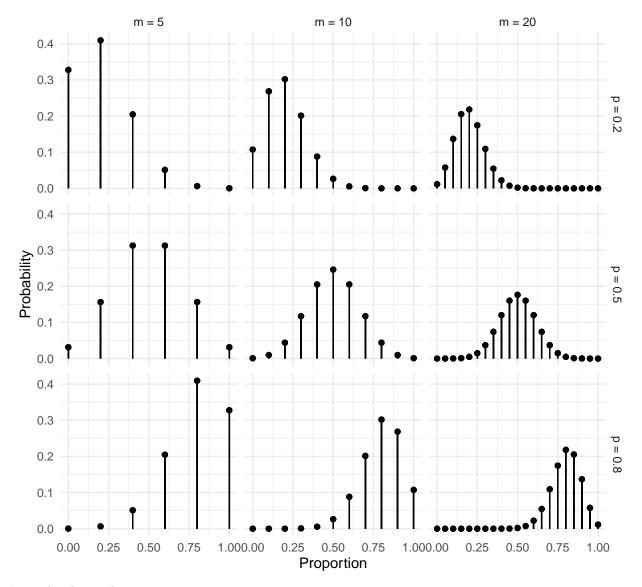
Outcome	Probability	
SSSF	$0.2 \times 0.2 \times 0.2 \times 0.8$	
SSFS	$0.2\times0.2\times0.2\times0.8$	
SFSS	$0.2\times0.2\times0.2\times0.8$	
FSSS	$0.2\times0.2\times0.2\times0.8$	

The proportion is obtained as Y = C/m.

The figures below show several binomial distributions for different values of m and p.



The figures below show the distributions of the proportion C/m.



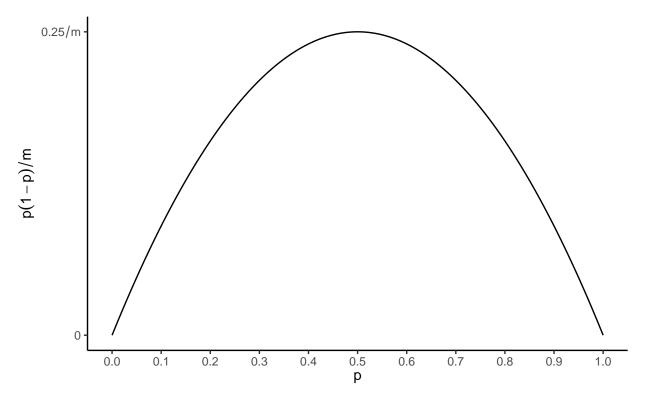
It can be shown that

$$E(C) = mp$$
 and $Var(C) = mp(1-p)$.

Then for the proportion Y = C/m it follows that

$$E(Y) = p$$
 and $Var(Y) = p(1-p)/m$.

This is because E(Y) = E(C/m) = E(C)/m = mp/m = p and $Var(Y) = Var(C/m) = Var(C)/m^2 = mp(1-p)/m^2 = p(1-p)/m$. Note that the variance is at its maximum when p = 0.5 and gets smaller as p moves away from 0.5 toward p = 0 or p = 1.



An important special case of the binomial distribution is the *Bernoulli distribution* where m=1 so that C=0,1 and Y=0,1.

Binomial Generalized Linear Models

Assume that each C_1, C_2, \ldots, C_n has a binomial distribution with parameters p_1, p_2, \ldots, p_n and m_1, m_2, \ldots, m_n , respectively, but m_1, m_2, \ldots, m_n are observed/known). A binomial GLM will then specify the expected value of $Y_i = C_i/m_i$ as

$$g[E(Y_i)] = \eta_i$$
 or $E(Y_i) = g^{-1}(\eta_i)$,

where $\eta_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik}$.

Recall that $E(Y_i) = p_i$ so we are effectively specifying a model for the *probability of a success*. The variance of Y_i is then

$$Var(Y_i) = E(Y_i)[1 - E(Y_i)]/m_i = p_i(1 - p_i)/m_i,$$

so that $0 \leq \text{Var}(Y_i) \leq 0.25m_i$. Like rates, it is preferable to *not* model proportions as response variables without accounting for the denominator m_i since it affects the variance.

Logistic Regression

Logistic regression is a binomial generalized linear model that uses a "logit" link function such that

$$g[E(Y_i)] = \log\left[\frac{E(Y_i)}{1 - E(Y_i)}\right] = \log\left(\frac{p_i}{1 - p_i}\right),$$

and therefore

$$E(Y_i) = \frac{e^{\eta_i}}{1 + e^{\eta_i}}$$
 or $p_i = \frac{e^{\eta_i}}{1 + e^{\eta_i}}$,

where again $\eta_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik}$. Note that this guarantees that $0 < E(Y_i) < 1$.

Example: Consider again the bliss data. The glm function can be used to estimate the logistic regression model where

$$E(Y_i) = \frac{e^{\eta_i}}{1 + e^{\eta_i}},$$

where $\eta_i = \beta_0 + \beta_1 x_i$ and x_i is the concentration for the *i*-th observation (i.e., the *i*-th batch of beetles).

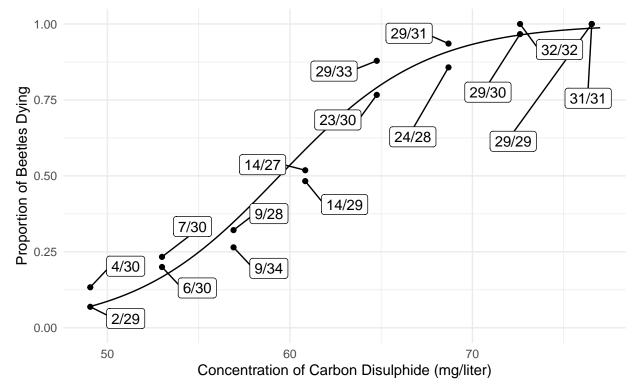
```
m <- glm(cbind(dead, exposed - dead) ~ concentration,
  family = binomial(link = logit), data = bliss)
cbind(summary(m)$coefficients, confint(m))</pre>
```

```
Estimate Std. Error z value Pr(>|z|) 2.5 % 97.5 % (Intercept) -14.8084 1.28976 -11.48 1.633e-30 -17.4785 -12.4089 concentration 0.2492 0.02138 11.65 2.250e-31 0.2095 0.2935
```

Here the two variables in cbind are the number of times the event occurred (i.e., C_i) and the number of times the event did not occur (i.e., $m_i - C_i$). If the variables had been dead and alive, representing the number of dead and alive beetles, respectively, then we'd write cbind(dead, alive). Also for family = binomial the logit link function is the default so you can use family = binomial for logistic regression.

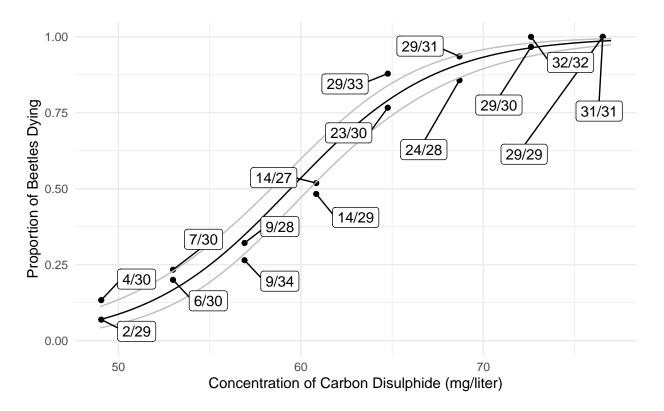
```
d <- data.frame(concentration = seq(49, 77, length = 1000))
d$yhat <- predict(m, newdata = d, type = "response")

p <- ggplot(bliss, aes(x = concentration, y = dead/exposed)) +
    geom_point() + ylim(0, 1) + theme_minimal() +
    geom_line(aes(y = yhat), data = d) +
    geom_label_repel(aes(label = proportion), box.padding = 0.75) +
    labs(x = "Concentration of Carbon Disulphide (mg/liter)",
        y = "Proportion of Beetles Dying")
plot(p)</pre>
```



Predicted probabilities, with confidence intervals, can also be obtained using contrast or glmint. Note that the function $e^x/(1+e^x)$ is known to R as plogis.

```
trtools::contrast(m, list(concentration = c(50,60,70)),
  cnames = c("50 mg/liter","60 mg/liter","70 mg/liter"), tf = plogis)
            estimate lower upper
50 mg/liter 0.08707 0.05512 0.1349
60 mg/liter 0.53539 0.47121 0.5984
70 mg/liter 0.93299 0.89490 0.9579
trtools::glmint(m, newdata = data.frame(concentration = c(50,60,70)))
      fit
              low
                     upp
1 0.08707 0.05512 0.1349
2 0.53539 0.47121 0.5984
3 0.93299 0.89490 0.9579
d <- data.frame(concentration = seq(49, 77, length = 1000))</pre>
d <- cbind(d, trtools::glmint(m, newdata = d))</pre>
head(d)
  concentration
                    fit
                            low
         49.00 0.06920 0.04201 0.1119
1
         49.03 0.06965 0.04233 0.1125
3
          49.06 0.07010 0.04266 0.1131
4
          49.08 0.07056 0.04299 0.1137
5
          49.11 0.07102 0.04332 0.1143
          49.14 0.07148 0.04365 0.1149
p <- ggplot(bliss, aes(x = concentration, y = dead/exposed)) +</pre>
  geom_point() + ylim(0, 1) + theme_minimal() +
  geom_line(aes(y = fit), data = d) +
  geom\_line(aes(y = low), data = d, color = grey(0.75)) +
  geom_line(aes(y = upp), data = d, color = grey(0.75)) +
  geom_label_repel(aes(label = proportion), box.padding = 0.75) +
  labs(x = "Concentration of Carbon Disulphide (mg/liter)",
    y = "Proportion of Beetles Dying")
plot(p)
```



Parameter and Contrast Interpretation: Odds Ratios

A logistic regression model can be written as

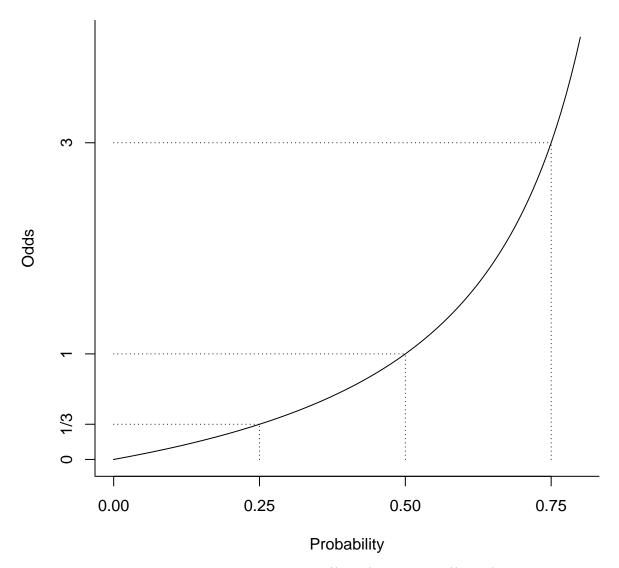
$$\frac{p_i}{1 - p_i} = \exp(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik})$$

where $p_i/(1-p_i)$ is the odds of the event. The odds is simply the ratio of the probability of the event occurring (p_i) to the probability of the event not occurring $(1-p_i)$.

Odds are sometimes stated in "fractional form" as two numbers separated by a colon or other character (e.g., an odds of 1.5 might be written as "3:2" or "three to two"). Note that in its fractional form the odds a:b implies a probability of a/(a+b).

	Odds	
Probability	Numeric	Fractional
0.01	0.01	1:99
0.1	0.11	1:9
0.25	0.33	1:3
1/3	0.50	1:2
0.4	0.67	2:3
0.5	1.00	1:1
0.6	1.50	3:2
2/3	2.00	2:1
0.75	3.00	3:1
0.9	9.00	9:1
0.99	99.00	99:1

It is important to note that probabilities and odds are related but not equal.



Let O_i be the odds for the *i*-th observation. Then $O_i = p_i/(1-p_i)$ and $p_i = O_i/(1+O_i)$. Note that $0 \le p_i \le 1$ but $0 \le O_i \le \infty$.

We can write a logistic regression model in terms of the odds of an event as

$$O_i = \exp(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik}),$$

or

$$O_i = e^{\beta_0} e^{\beta_1 x_{i1}} e^{\beta_2 x_{i2}} \cdots e^{\beta_k x_{ik}}.$$

Here we can use contrast to make inferences about the odds of death.

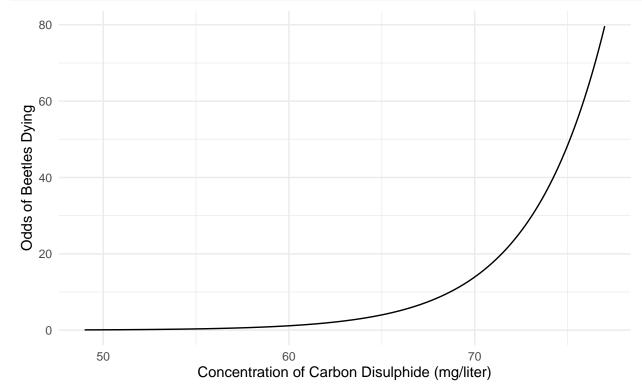
```
trtools::contrast(m, list(concentration = c(50,60,70)),
  cnames = c("50 mg/liter","60 mg/liter","70 mg/liter"), tf = exp)
```

```
estimate lower upper 50 mg/liter 0.09538 0.05833 0.1559 60 mg/liter 1.15232 0.89110 1.4901 70 mg/liter 13.92222 8.51430 22.7650
```

We can even plot the estimated odds of death.

```
d <- data.frame(concentration = seq(49, 77, length = 1000))
d$yhat <- predict(m, newdata = d, type = "response")
d$odds <- d$yhat / (1 - d$yhat)

p <- ggplot(d, aes(x = concentration, y = odds)) +
    geom_line() + theme_minimal() +
    labs(x = "Concentration of Carbon Disulphide (mg/liter)",
        y = "Odds of Beetles Dying")
plot(p)</pre>
```



The model for the odds is "log-linear" like the model for expected counts in Poisson regression. To interpret the parameters of a logistic regression model, we can use *odds ratios* which are similar to rate ratios in Poisson regression.

Odds Ratio: Quantitative Explanatory Variable

Suppose we have the logistic regression model

$$O_i = \exp(\beta_0 + \beta_1 x) = e^{\beta_0} e^{\beta_1 x},$$

were x_i is a quantitative explanatory variable. Consider the odds at x and x + 1 for arbitrary x,

$$O_a = e^{\beta_0} e^{\beta_1(x+1)}$$
 and $O_b = e^{\beta_0} e^{\beta_1 x}$.

Then the odds ratio is

$$\frac{O_a}{O_b} = \frac{e^{\beta_0}e^{\beta_1(x+1)}}{e^{\beta_0}e^{\beta_1x}} = \frac{e^{\beta_0}e^{\beta_1x}e^{\beta_1}}{e^{\beta_0}e^{\beta_1x}} = e^{\beta_1} \Leftrightarrow O_a = O_be^{\beta_1},$$

so that an increase x by one unit changes the odds by a factor of e^{β_1} . Also, we can compute the percent change in the odds as

$$100\% \times [O_a/O_b - 1],$$

where $O_a/O_b = e^{\beta_1}$ is the odds ratio. Again, the sign tells us if this is a percent increase or decrease in the odds.

Example: Consider again the model for the bliss data.

```
cbind(summary(m)$coefficients, confint(m))
              Estimate Std. Error z value Pr(>|z|)
                                                        2.5 %
                                                                 97.5 %
              -14.8084
                          1.28976 -11.48 1.633e-30 -17.4785 -12.4089
(Intercept)
concentration
                0.2492
                           0.02138
                                     11.65 2.250e-31
                                                       0.2095
                                                                 0.2935
exp(cbind(coef(m), confint(m)))
                             2.5 %
                                      97.5 %
              3.705e-07 2.566e-08 4.082e-06
(Intercept)
concentration 1.283e+00 1.233e+00 1.341e+00
trtools::contrast(m, tf = exp,
 a = list(concentration = 2),
 b = list(concentration = 1))
 estimate lower upper
    1.283 1.23 1.338
An odds ratio is then simply the ratio of the odds at two different values of an explanatory variable. We
could compute the odds ratio, for example, for an increase of 1, 5, 10, and 20 mg/liter.
trtools::contrast(m, tf = exp,
  a = list(concentration = c(1,5,10,20)),
  b = list(concentration = 0),
  cnames = c("+1 mg/liter", "+5 mg/liter", "+10 mg/liter", "+20 mg/liter"))
             estimate lower
                               upper
+1 mg/liter
                1.283 1.230
                                1.338
+5 mg/liter
                3.476 2.819
                               4.286
+10 mg/liter
              12.082 7.945 18.372
+20 mg/liter 145.971 63.126 337.540
Suppose that we model instead the probability of survival rather than death.
m <- glm(cbind(exposed - dead, dead) ~ concentration,
 family = binomial, data = bliss)
cbind(summary(m)$coefficients, confint(m))
              Estimate Std. Error z value Pr(>|z|)
                                                       2.5 % 97.5 %
(Intercept)
               14.8084
                          1.28976
                                    11.48 1.633e-30 12.4089 17.4785
concentration -0.2492
                          0.02138 -11.65 2.250e-31 -0.2935 -0.2095
exp(cbind(coef(m), confint(m)))
                             2.5 %
              2.699e+06 2.450e+05 3.898e+07
(Intercept)
concentration 7.794e-01 7.456e-01 8.110e-01
trtools::contrast(m, tf = exp,
 a = list(concentration = 2),
 b = list(concentration = 1))
 estimate lower upper
  0.7794 0.7475 0.8128
```

Note the "symmetry" of logistic regression. Whether we model the probability of the event or its complement is just a matter of parameterization.

Odds Ratio: Categorical Explanatory Variable

Suppose we have the model

$$O_i = \exp(\beta_0 + \beta_1 x) = e^{\beta_0} e^{\beta_1 x}.$$

were x is an indicator variable so that

$$x = \begin{cases} 1, & \text{if the observation is from group } a, \\ 0, & \text{if the observation is from group } b, \end{cases}$$

so that the model can be written as

$$O_i = \begin{cases} e^{\beta_0} e^{\beta_1}, & \text{if the observation is from group } a, \\ e^{\beta_0}, & \text{if the observation is from group } b. \end{cases}$$

So we can write the odds as

$$O_a = e^{\beta_0} e^{\beta_1}$$
 and $O_b = e^{\beta_0}$.

The odds ratio is then

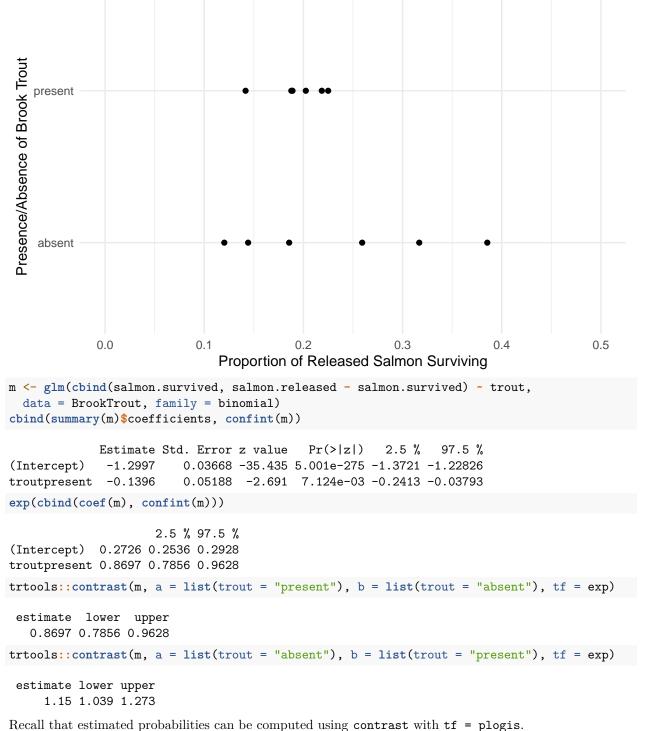
$$\frac{O_a}{O_b} = \frac{e^{\beta_0}e^{\beta_1}}{e^{\beta_0}} = e^{\beta_1} \quad \text{or} \quad \frac{O_b}{O_a} = \frac{e^{\beta_0}}{e^{\beta_0}e^{\beta_1}} = \frac{1}{e^{\beta_1}} = e^{-\beta_1}.$$

So the odds for group a is e^{β_1} times that for group b, and the odds for group b is $e^{-\beta_1} = 1/e^{\beta_1}$ times that for group a. We can compute how much larger (or smaller) O_a is relative to O_b with

$$100\% \times [O_a/O_b - 1],$$

where $O_a/O_b = e^{\beta_1}$ is the odds ratio. The sign tells us if O_a is a percent larger or smaller than O_b .

Example: Consider the following data from a study that investigated the effect of non-indigenous brook trout on the survival of salmon.



Recan that estimated probabilities can be computed using contrast with tr - progrs

```
trtools::contrast(m, a = list(trout = c("present", "absent")),
    tf = plogis, cnames = c("prob @ present", "prob @ absent"))
```

Similarly the estimated odds can be computed if tf = exp.

```
trtools::contrast(m, a = list(trout = c("present", "absent")),
    tf = exp, cnames = c("odds @ present", "odds @ absent"))
```

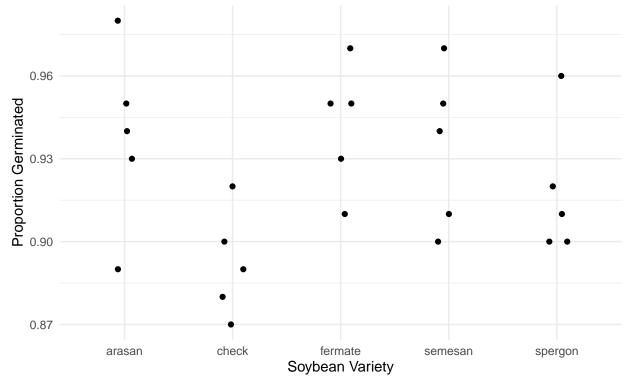
The odds ratios are then simply a ratio of these odds.

Example: Consider the following study of the germination of five varieties of soybean seeds. Note that each observation was the number of seeds that *failed* to germinate out of 100 seeds.

```
head(faraway::soybean)
```

```
variety replicate failure
1
    check
                   1
                   2
2
    check
                           10
3
    check
                   3
                           12
    check
                    4
                           13
4
5
    check
                   5
                           11
  arasan
                    1
```

```
p <- ggplot(faraway::soybean, aes(x = variety, y = (100-failure)/100)) +
  geom_jitter(height = 0, width = 0.1) + theme_minimal() +
  labs(x = "Soybean Variety", y = "Proportion Germinated")
plot(p)</pre>
```



```
m <- glm(cbind(100 - failure, failure) ~ variety, family = binomial, data = faraway::soybean)
exp(cbind(coef(m), confint(m)))</pre>
```

```
2.5 % 97.5 % (Intercept) 15.1290 10.7107 22.2134
```

```
varietycheck
               0.5459 0.3412 0.8594
varietyfermate 1.0735 0.6361 1.8167
varietysemesan 0.9354 0.5616 1.5542
varietyspergon 0.7400 0.4531 1.1972
# compute odds ratio of germination for arasan, fermate, semesan, and spergon versus check
trtools::contrast(m, tf = exp,
 a = list(variety = c("arasan", "fermate", "semesan", "spergon")),
 b = list(variety = "check"),
 cnames = c("arasan/check","fermate/check","semesan/check","spergon/check"))
             estimate lower upper
                1.832 1.1560 2.902
arasan/check
fermate/check
                1.966 1.2297 3.145
semesan/check
              1.713 1.0902 2.693
spergon/check
                1.355 0.8849 2.076
Aggregated Versus Binary Responses
```

Suppose the observations in the bliss data were for individual beetles.

```
blissbin <- bliss %>% mutate(alive = exposed - dead) %>%
  select(concentration, dead, alive) %>%
  pivot_longer(cols = c(dead,alive), names_to = "state", values_to = "count") %>%
 uncount(count)
head(blissbin)
```

```
# A tibble: 6 x 2
  concentration state
          <dbl> <chr>
           49.1 dead
1
           49.1 dead
2
3
           49.1 alive
           49.1 alive
4
           49.1 alive
5
6
           49.1 alive
```

We can specify the response variable as follows.

```
m <- glm(state == "dead" ~ concentration, family = binomial, data = blissbin)
summary(m)$coefficients
```

```
Estimate Std. Error z value Pr(>|z|)
(Intercept)
             -14.8084
                       1.28972 -11.48 1.627e-30
concentration 0.2492
                         0.02138
                                  11.65 2.241e-31
```

Of if the response variable is binary we can specify the model as follows.

```
blissbin <- blissbin %>% mutate(y = ifelse(state == "dead", 1, 0))
m <- glm(y ~ concentration, family = binomial, data = blissbin)
summary(m)$coefficients
```

```
Estimate Std. Error z value Pr(>|z|)
             -14.8084 1.28972 -11.48 1.627e-30
(Intercept)
concentration 0.2492
                         0.02138
                                   11.65 2.241e-31
m <- glm(cbind(y, 1-y) ~ concentration, family = binomial, data = blissbin)</pre>
summary(m)$coefficients
```

```
Estimate Std. Error z value Pr(>|z|) (Intercept) -14.8084 1.28972 -11.48 1.627e-30 concentration 0.2492 0.02138 11.65 2.241e-31
```

Note that our parameter estimates and other inferences are the same as what we obtained with the aggregated data.

head(bliss)

```
concentration dead exposed proportion
          49.06
                            29
          49.06
                                     4/30
2
                            30
3
          52.99
                    7
                            30
                                     7/30
4
          52.99
                            30
                                     6/30
                    6
5
          56.91
                                     9/28
                    9
                            28
6
          56.91
                    9
                            34
                                     9/34
m <- glm(cbind(dead, exposed - dead) ~ concentration,
  family = binomial, data = bliss)
```

It is usually not necessary to transform aggregate data into binary data, but it is sometimes useful to transform binary data into aggregate data. Here is how that can be done. Note that any explanatory variables (separated by commas) are listed in group_by and the response variable is listed in count.

```
blissagg <- blissbin %>% group_by(concentration) %>% count(state) %>%
  pivot_wider(names_from = state, values_from = n, values_fill = 0)
blissagg
```

```
# A tibble: 8 x 3
# Groups:
            concentration [8]
  concentration alive dead
          <dbl> <int> <int>
1
            49.1
                    53
2
           53.0
                    47
                           13
3
           56.9
                    44
                           18
4
           60.8
                    28
                           28
5
            64.8
                    11
                           52
6
            68.7
                     6
                           53
7
           72.6
                     1
                           61
           76.5
8
                     0
                           60
```

```
m <- glm(cbind(dead, alive) ~ concentration, family = binomial, data = blissagg)
summary(m)$coefficients</pre>
```

```
Estimate Std. Error z value Pr(>|z|) (Intercept) -14.8084 1.28976 -11.48 1.633e-30 concentration 0.2492 0.02138 11.65 2.250e-31
```