Logistic Regression (Part III)

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Variations of logistic regression

Logistic regression

- In logistic regression, we use the logit:

$$\text{logit}\left(p\right) = x^{\top}\beta = \eta$$

  which results in

$$p = \left[1 + \exp\left(-\eta\right)\right]^{-1} = F\left(\eta\right)$$

- Technically, F can be any *monotonic* function that maps η to $[0, 1]$ (e.g., any CDF will work)
- F^{-1} is called the link function

The probit model

- The probit model uses $F\left(\eta\right) = \Phi\left(\eta\right)$ (i.e., the CDF of a standard normal distribution)

$$P\left(Y = 1|x\right) = \Phi\left(\beta_0 + \beta_1 x_1 + \cdots\right) = \Phi\left(x^{\top}\beta\right)$$

- $F^{-1} = \Phi^{-1}$ is called the probit link, which yields

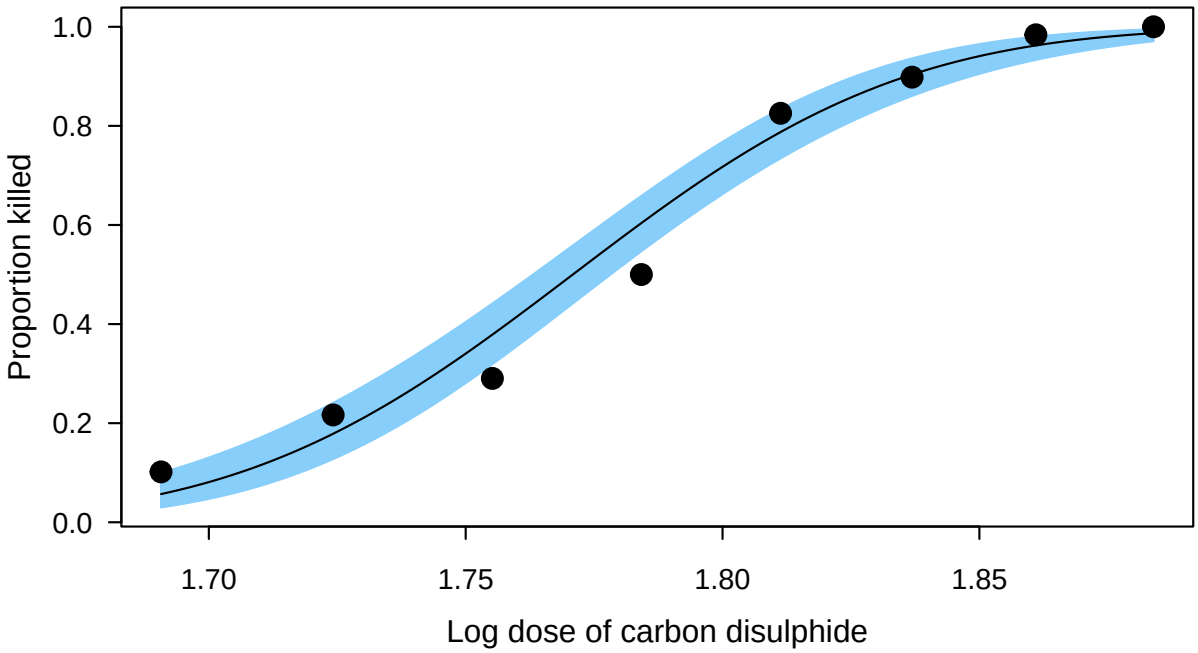
$$\text{probit}\left(p\right) = \Phi^{-1}\left(p\right) = x^{\top}\beta$$

- The term probit is short for **prob**ability un**it**
- Proposed in Bliss (1934) for analyzing data such as the percentage of a pest killed by a pesticide

Dobson's beetle data

The data give the number of flour beetles killed after five hour exposure to the insecticide carbon disulphide at eight different concentrations.

```
beetle <- investr::beetle
fit <- glm(cbind(y, n-y) ~ ldose, data = beetle,
           family = binomial(link = "probit"))
investr::plotFit(
  fit, pch = 19, cex = 1.2, lwd = 2,
  xlab = "Log dose of carbon disulphide", ylab = "Proportion killed",
  interval = "confidence", shade = TRUE, col.conf = "lightskyblue"
)
```



Other link functions

Common link function for binary regression include:

- Logit (most common and the default an most software)
- Probit (next most common)
- Log-log
- Complimentary log-log

- Cauchit

Application to wcgs data set

Comparing coefficients from different link functions:

```
wcgs <- na.omit(subset(faraway::wcgs, select = -c(typechd, timechd, behave)))

# Fit binary GLMs with different link functions
fit.logit <- glm(chd ~ ., data = wcgs, family = binomial(link = "logit"))
fit.probit <- glm(chd ~ ., data = wcgs, family = binomial(link = "probit"))
fit.cloglog <- glm(chd ~ ., data = wcgs, family = binomial(link = "cloglog"))
fit.cauchit <- glm(chd ~ ., data = wcgs, family = binomial(link = "cauchit"))

# Compare coefficients
coefs <- cbind(
  "logit" = coef(fit.logit),
  "probit" = coef(fit.probit),
  "cloglog" = coef(fit.cloglog),
  "cauchit" = coef(fit.cauchit)
)
round(coefs, digits = 3)
```

```
               logit probit cloglog cauchit
(Intercept)  -12.246 -6.452 -11.377 -24.086
age            0.062  0.031   0.057   0.115
height         0.007  0.003   0.007   0.053
weight         0.009  0.005   0.007   0.003
sdp            0.018  0.010   0.017   0.042
dbp           -0.001 -0.001  -0.001  -0.001
chol           0.011  0.006   0.010   0.020
cigs           0.021  0.011   0.019   0.043
dibepB        -0.658 -0.341  -0.604  -1.320
arcuspresent   0.211  0.101   0.206   0.711
```

Application to wcgs data set

Comparing fitted values from different link functions:

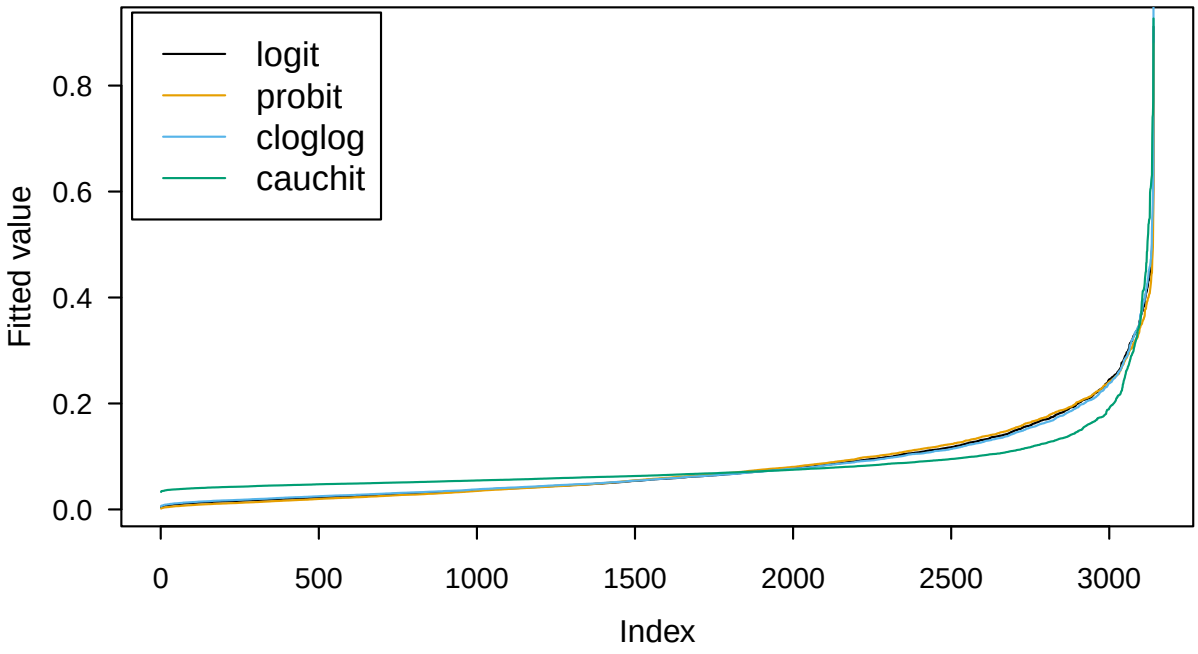
```r
# Compare fitted values (i.e., predicted probabilities)
preds <- cbind(
  "logit" = fitted(fit.logit),
  "probit" = fitted(fit.probit),
  "cloglog" = fitted(fit.cloglog),
  "cauchit" = fitted(fit.cauchit)
)
head(round(preds, digits = 3))
```

```
  logit probit cloglog cauchit
1 0.071  0.072   0.072   0.076
2 0.073  0.074   0.075   0.084
3 0.010  0.006   0.011   0.038
4 0.010  0.006   0.012   0.039
5 0.169  0.167   0.168   0.150
6 0.034  0.033   0.035   0.051
```

Application to wcgs data set

Comparing fitted values from different link functions:

```r
plot(sort(preds[, "logit"]), type = "l", ylab = "Fitted value")
lines(sort(preds[, "probit"]), col = 2)
lines(sort(preds[, "cloglog"]), col = 3)
lines(sort(preds[, "cauchit"]), col = 4)
legend("topleft", legend = c("logit", "probit", "cloglog", "cauchit"),
       col = 1:4, lty = 1, inset = 0.01)
```



As a latent variable model

- Logistic regression (and the other link functions) has an equivalent formulation as a latent variable model
- Consider a linear model with continuous outcome $Y^\star = x^\top \beta + \epsilon$
- Imagine that we can only observe the binary variable

$$Y = \begin{cases} 1 & \text{if } Y^\star > 0, \\ 0 & \text{otherwise} \end{cases}$$

- Assuming $\epsilon \sim \text{Logistic}\,(0, 1)$ leads to the usual logit model
- Assuming $\epsilon \sim N\,(0, 1)$ leads to the probit model
- And so on...

Application: surrogate residual

- There are several types of residuals defined for logistic regression (e.g., deviance residuals and Pearson residuals)
- The surrogate residual act like the usual residual from a normal linear model and has similar properties!

- See Liu and Zhang (2018), Greenwell et al. (2018), and Cheng et al. (2020) for details
- A novel R-squared measure based on the surrogate idea was proposed in Liu et al. (2022)
- For implementation, see R packages sure, SurrogateRsq, and PAsso

Binomial data

O-rings example

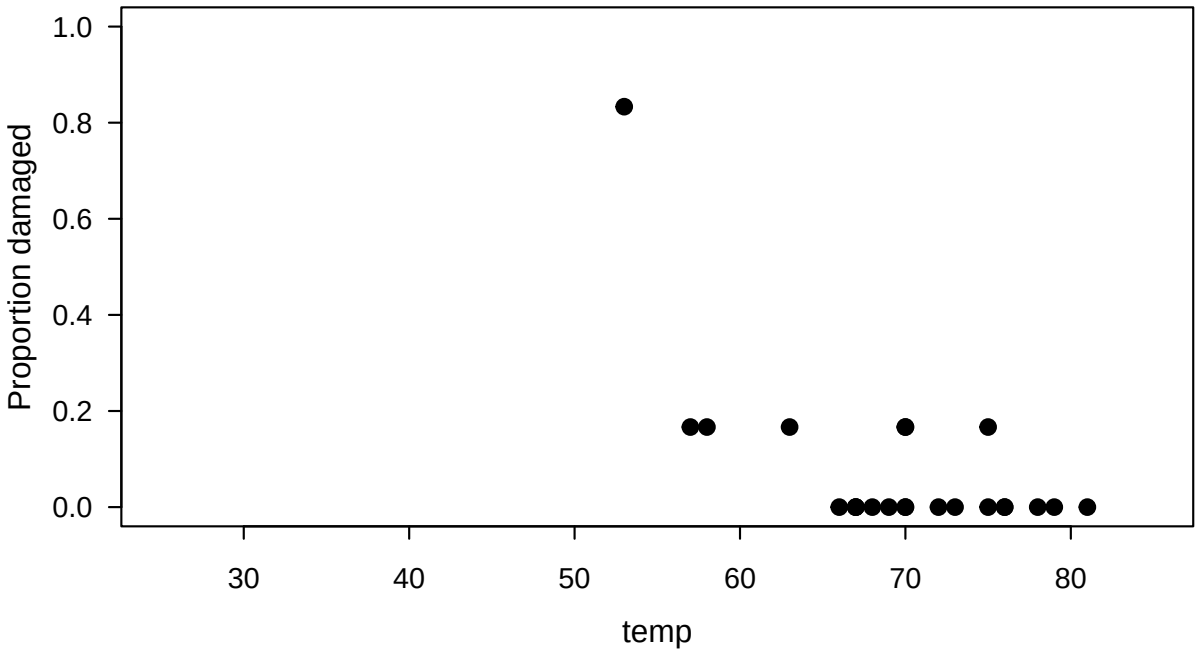
On January 28, 1986, the Space Shuttle Challenger broke apart 73 seconds into its flight, killing all seven crew members aboard. The crash was linked to the failure of O-ring seals in the rocket engines. Data was collected on the 23 previous shuttle missions. The launch temperature on the day of the crash was 31 °F.

```
head(orings <- faraway::orings)
```

```
  temp damage
1   53      5
2   57      1
3   58      1
4   63      1
5   66      0
6   67      0
```

O-rings example

```
plot(damage/6 ~ temp, data = orings, xlim = c(25, 85), pch = 19,
     ylim = c(0, 1), ylab = "Proportion damaged")
```



O-rings example

Expand binomial data into independent Bernoulli trials

```
tmp <- rep(orings$temp, each = 6)
dmg <- sapply(orings$damage, FUN = function(x) rep(c(0, 1), times = c(6 - x, x)))
orings2 <- data.frame("temp" = tmp, "damage" = as.vector(dmg))
head(orings2, n = 15)
```

```
   temp damage
1    53      0
2    53      1
3    53      1
4    53      1
5    53      1
6    53      1
7    57      0
8    57      0
9    57      0
10   57      0
11   57      0
12   57      1
```

```
13   58      0
14   58      0
15   58      0
```

O-rings example

Here we'll just fit a logistic regression to the expanded bernoulli version of the data

```
# Fit a logistic regression (LR) model using 0/1 version of the data
orings.lr <- glm(damage ~ temp, data = orings2,
                 family = binomial(link = "logit"))
summary(orings.lr)
```

```
Call:
glm(formula = damage ~ temp, family = binomial(link = "logit"),
    data = orings2)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.2646  -0.3395  -0.2472  -0.1299   3.0216

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) 11.66299    3.29616   3.538 0.000403 ***
temp        -0.21623    0.05318  -4.066 4.77e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 76.745  on 137  degrees of freedom
Residual deviance: 54.759  on 136  degrees of freedom
AIC: 58.759

Number of Fisher Scoring iterations: 6
```

O-rings example

What's the estimated probability that an O-ring will be damaged at 31 °F? Give a point estimate as well as a 95% confidence interval.

. . .

```
predict(orings.lr, newdata = data.frame("temp" = 31), type = "response",
        se = TRUE)
```

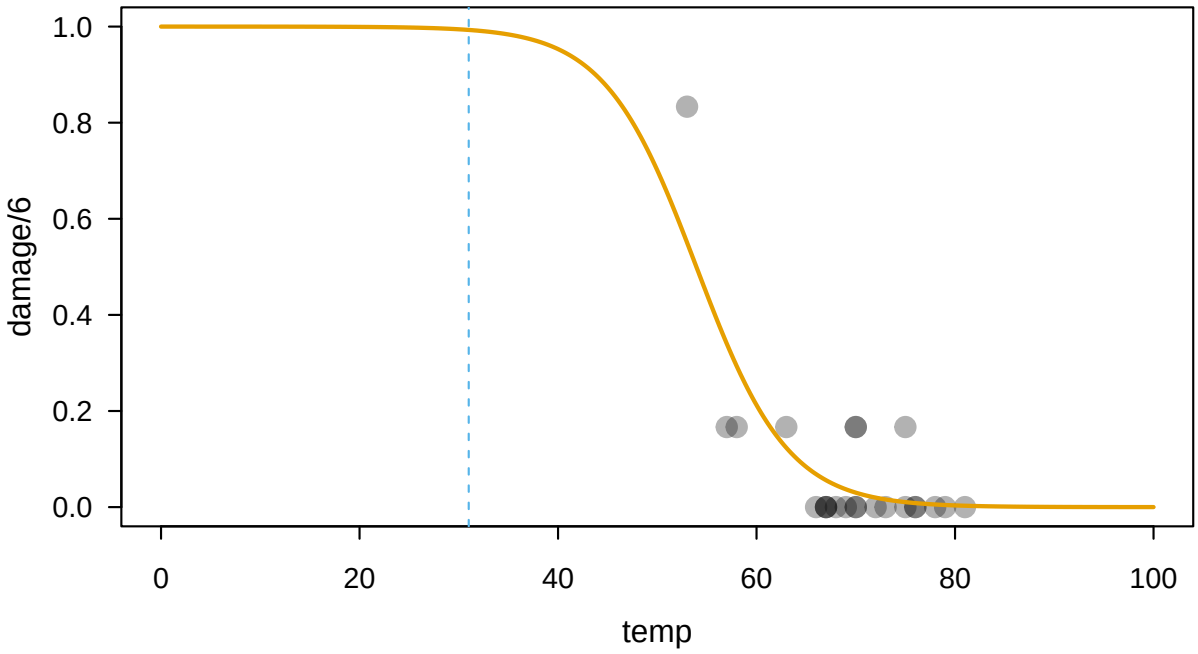
```
$fit
        1
0.9930342

$se.fit
         1
0.01153302

$residual.scale
[1] 1
```

```
# Better approach for a 95% CI?
pred <- predict(orings.lr, newdata = data.frame("temp" = 31),
                type = "link", se = TRUE)
plogis(pred$fit + c(-qnorm(0.975), qnorm(0.975)) * pred$se.fit)
```

```
[1] 0.8444824 0.9997329
```

O-rings example

```
# Is this extrapolating?
plot(damage / 6 ~ temp, data = orings, pch = 19, cex = 1.3,
     col = adjustcolor(1, alpha.f = 0.3), xlim = c(0, 100), ylim = c(0, 1))
x <- seq(from = 0, to = 100, length = 1000)
y <- predict(orings.lr, newdata = data.frame("temp" = x),
             type = "response")
lines(x, y, lwd = 2, col = 2)
abline(v = 31, lty = 2, col = 3)
```



O-rings examples

More interesting question: at what temperature(s) can we expect the risk/probability of damage to exceed 0.8?

. . .

This is a problem of inverse estimation, which is the purpose of the investr package!

```
# To install from CRAN, use
#
# > install.packages("investr")
#
# See ?investr::invest for details and examples
investr::invest(orings.lr, y0 = 0.8, interval = "Wald", lower = 40, upper = 60)
```

```
 estimate     lower     upper        se
47.525881 39.993462 55.058299  3.843141
```

O-rings example

Here's an equivalent logistic regression model fit to the original binomial version of the data (need to provide number of successes and number of failures)

```r
orings.lr2 <- glm(cbind(damage, 6 - damage) ~ temp, data = orings,
                  family = binomial(link = "logit"))
summary(orings.lr2)
```

```
Call:
glm(formula = cbind(damage, 6 - damage) ~ temp, family = binomial(link = "logit"),
    data = orings)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-0.9529  -0.7345  -0.4393  -0.2079   1.9565

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) 11.66299    3.29626   3.538 0.000403 ***
temp        -0.21623    0.05318  -4.066 4.78e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 38.898  on 22  degrees of freedom
Residual deviance: 16.912  on 21  degrees of freedom
AIC: 33.675

Number of Fisher Scoring iterations: 6
```

Overdispersion

Overdispersion

Overdispersion

- Recall that for a Bernoulli random variable Y the mean and variance are given by $E(Y) = p$ and $V(Y) = p(1-p)$
- In other words, once the mean is specified by the logistic regression, the variance is determined at the same time!
- This is different from the case of linear regression models
- Sometimes the data suggest that the variance is consistently greater than $p(1-p)$

- Including a dispersion parameter can make the model more flexible: $V(Y) = \sigma^2 p(1-p)$

Overdispersion

- Over-dispersion is said to exist when there is more variability than expected under the response distribution; similar for underdispersion.
- For a correctly specified model, the Pearson chi-square statistic and the deviance, divided by their degrees of freedom, should be approximately equal to one. When their values are much larger than one, the assumption of binomial variability might not be valid and the data are said to exhibit overdispersion. Underdispersion, which results in the ratios being less than one, occurs less often in practice.

Overdispersion

- Overall performance of the fitted model can be measured by several different goodness-of-fit tests. Two tests that require replicated data (multiple observations with the same values for all the predictors) are the Pearson chi-square goodness-of-fit test and the deviance goodness-of-fit test (analagous to the multiple linear regression lack-of-fit F-test).
- When fitting a model, there are several problems that can cause the goodness-of-fit statistics to exceed their degrees of freedom. Among these are such problems as outliers in the data, using the wrong link function, omitting important terms from the model, and needing to transform some predictors. These problems should be eliminated before proceeding to use the following methods to correct for overdispersion.
- A large difference between the Pearson statistic and the deviance provides some evidence that the data are too sparse to use either statistic.

O-rings example

You can check for overdispersion manually or by using performance:

```
performance::check_overdispersion(orings.lr2)
```

```
# Overdispersion test

       dispersion ratio =  1.337
  Pearson's Chi-Squared = 28.067
              p-value =  0.138
```

Overdispersion

Two common (but equivalent) ways to handle overdispersion in R:

1. Estimate the dispersion parameter σ^2 and provide it to `summary()` to adjust the standard errors approriately
2. Use the `quasibinomial()` family

Overdispersion

Estimate the dispersion parameter σ^2; analagous to MSE in linear regression

```
(sigma2 <- sum(residuals(orings.lr2, type = "pearson") ^ 2) / orings.lr2$df.residual)
```

```
[1] 1.336542
```

```
# Print model summary based on estimated dispersion parameter
summary(orings.lr2, dispersion = sigma2)
```

```
Call:
glm(formula = cbind(damage, 6 - damage) ~ temp, family = binomial(link = "logit"),
    data = orings)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-0.9529  -0.7345  -0.4393  -0.2079   1.9565

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) 11.66299    3.81077   3.061 0.002209 **
temp        -0.21623    0.06148  -3.517 0.000436 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1.336542)

    Null deviance: 38.898  on 22  degrees of freedom
Residual deviance: 16.912  on 21  degrees of freedom
AIC: 33.675

Number of Fisher Scoring iterations: 6
```

Overdispersion

Can use `quasibinomial()` family to account for over-dispersion automatically (notice the estimated coeficients don't change)

```
orings.qb <- glm(cbind(damage, 6 - damage) ~ temp, data = orings,
                 family = quasibinomial)
summary(orings.qb)
```

```
Call:
glm(formula = cbind(damage, 6 - damage) ~ temp, family = quasibinomial,
    data = orings)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-0.9529  -0.7345  -0.4393  -0.2079   1.9565

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 11.66299    3.81077   3.061  0.00594 **
temp        -0.21623    0.06148  -3.517  0.00205 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for quasibinomial family taken to be 1.336542)

    Null deviance: 38.898  on 22  degrees of freedom
Residual deviance: 16.912  on 21  degrees of freedom
AIC: NA

Number of Fisher Scoring iterations: 6
```

Generalized additive models (GAMs)

- $\text{logit}\left(p\right) = \beta_0 + f_1\left(x_1\right) + f_2\left(x_2\right) + \cdots + f_p\left(x_p\right)$
  - The f_i are referred to as *shape functions* or *term contributions* and are often modeled using *splines*
  - Can also include pairwise interactions of the form $f_{ij}\left(x_i, x_j\right)$

- **Easy to interpret** (e.g., just plot the individual shape functions)!
  - Interaction effects can be understood with heat maps, etc.
- **Modern GAMs**, called GA2Ms, automatically include relevant pairwise interaction effects

Explainable boosting machines (EBMs)

- EBM .darkblue[GA2M] + .green[Boosting] + .tomato[Bagging]
- Python library: interpret

Questions?