The Generalized Linear Model & Logistic Regression

Introduction to Data Science Lecture 4

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Outline

1. Generalized linear models
2. Logistic regression
3. Multinomial logistic regression
4. Classification via logistic regression

General Linear Model

So far, we've been discussing models with this form:

$$Y = \beta_0 + \sum_{p=1}^{P} \beta_p X_p + \varepsilon$$

This type of model is known as the *general linear model*.

- All flavors of linear regression are general linear models.
  - ANOVA
  - ANCOVA
  - Multilevel linear regression models

Components of the General Linear Model

We can break our model into pieces:

$$\eta = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

$$Y = \eta + \varepsilon$$

Because $\varepsilon \sim \mathrm{N}(0, \sigma^2)$, we can also write:

$$Y \sim \mathrm{N}(\eta, \sigma^2)$$

In this representation:

- η is the *systematic component* of the model
- The normal distribution, $\mathrm{N}(\cdot, \cdot)$, is the model's *random component*.

Components of the General Linear Model

The purpose of general linear modeling (i.e., regression modeling) is to build a model of the outcome's mean, μ_Y.

- In this case, $\mu_Y = \eta$.
- The systematic component defines the mean of Y.

The random component quantifies variability (i.e., error variance) around μ_Y.

- In the general linear model, we assume that this error variance follows a normal distribution.
- Hence the normal random component.

Generalized Linear Model

We can generalize the models we've been using in two important ways:

1. Allow for random components other than the normal distribution.
2. Allow for more complicated relations between μ_Y and η.
   - Allow: $g(\mu_Y) = \eta$

These extensions lead to the class of *generalized linear models* (GLMs).

Components of the Generalized Linear Model

The random component in a GLM can be any distribution from the so-called *exponential family*.

- The exponential family contains many popular distributions:
  - Normal
  - Binomial
  - Poisson
  - Many others...

The systematic component of a GLM is exactly the same as it is in general linear models:

$$\eta = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

Link Functions

In GLMs, η does not directly describe μ_Y.

- We first transform μ_Y via a *link function*.
- $g(\mu_Y) = \eta$

The link function allows GLMs for outcomes with restricted ranges without requiring any restrictions on the range of the $\{X_p\}$.

- For strictly positive Y, we can use a *log link*:

$$\ln(\mu_Y) = \eta.$$

- The general linear model employs the *identity link*:

$$\mu_Y = \eta.$$

Components of the Generalized Linear Model

Every GLM is built from three components:

1. The systematic component, η.
   - A linear function of the predictors, $\{X_p\}$.
   - Describes the association between $\mathbf{X}$ and Y.

2. The link function, $g(\mu_Y)$.
   - Transforms μ_Y so that it can take any value on the real line.

3. The random component, $P(Y|g^{-1}(\eta))$
   - The distribution of the observed Y.
   - Quantifies the error variance around η.

General Linear Model $\subset$ Generalized Linear Model

The general linear model is a special case of GLM.

1. Systematic component:

$$\eta = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

2. Link function:

$$\mu_Y = \eta$$

3. Random component:

$$Y \sim \mathrm{N}(\eta, \sigma^2)$$

Logistic Regression

Logistic Regression

So why do we care about the GLM when linear regression models have worked thus far?

- In a word: Classification.

In the classification task, we have a discrete, qualitative outcome.

- We will begin with the situation of two-level outcomes.
  - Alive or Dead
  - Pass or Fail
  - Pay or Default

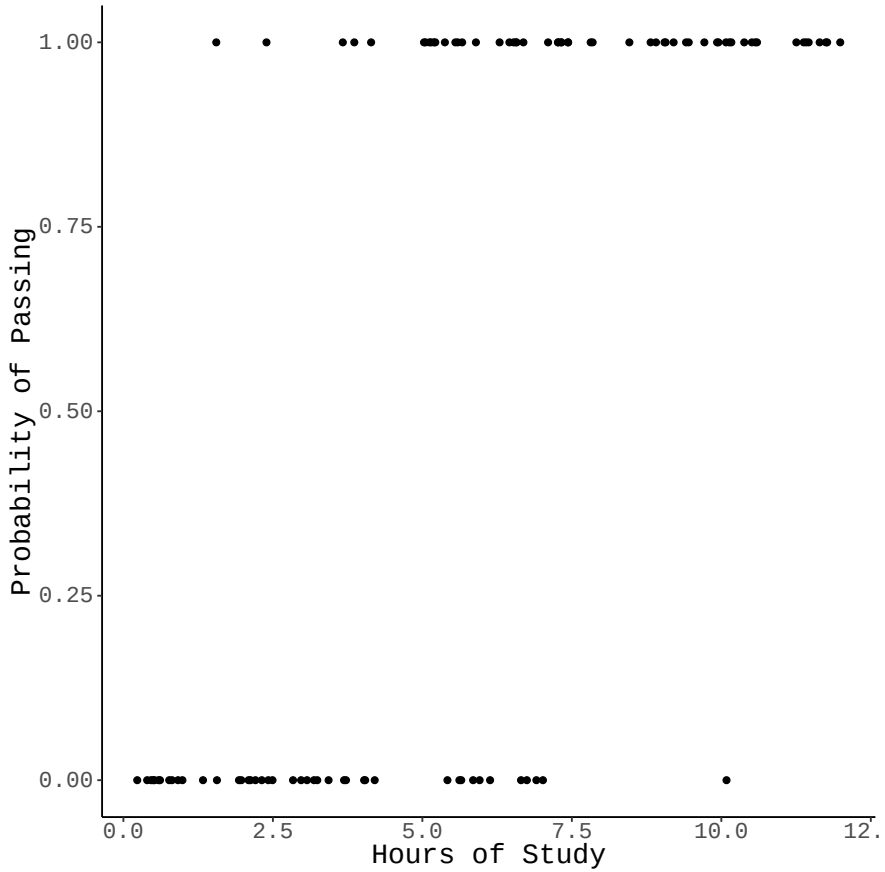
We want to build a model that predicts class membership based on some set of interesting features.

- To do so, we will use a very useful type of GLM: *logistic regression*.

Classification Example

Suppose we want to know the effect of study time on the probability of passing an exam.

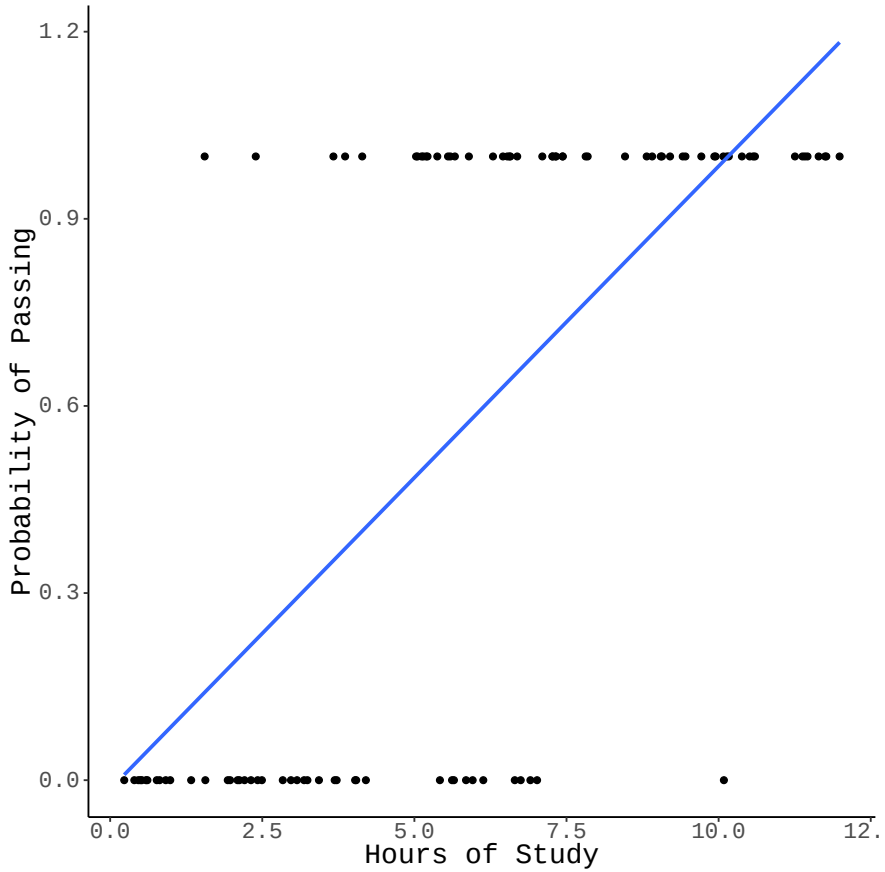
- The probability of passing must be between 0 and 1.
- We care about the probability of passing, but we only observe absolute success or failure.
  - $Y \in \{1, 0\}$



Linear Regression for Binary Outcomes?

What happens if we try to model these data with linear regression?

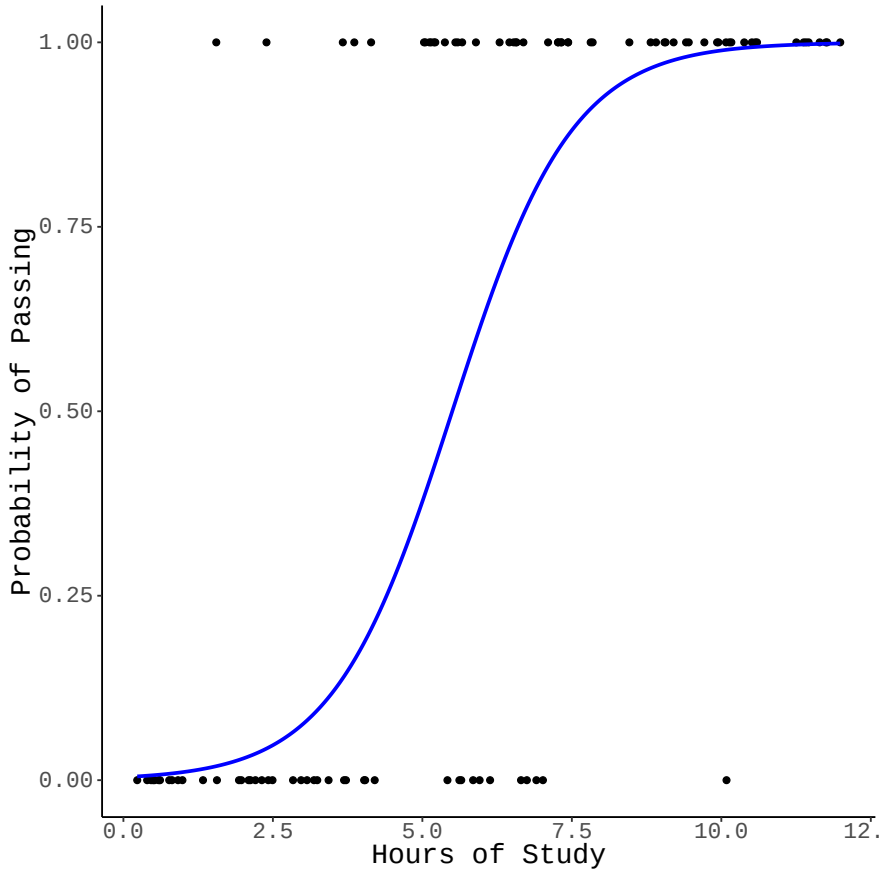
- Hmm...notice any problems?



Logistic Regression Visualized

We get a much better model using logistic regression.

- The link function ensures legal predicted values.
- The sigmoidal curve implies fluctuation in the effectiveness of extra study time.
  - More study time is most beneficial for students with around 5.5 hours of study.



Defining the Logistic Regression Model

In logistic regression problems, we are modeling binary data:

- Usual coding: $Y \in \{1 = \text{“Success”}, 0 = \text{“Failure”}\}$.

The *Binomial* distribution is a good way to represent this kind of data.

- The systematic component in our logistic regression model will be the binomial distribution.

The mean of the binomial distribution (with $N = 1$) is the “success” probability, $\pi = P(Y = 1)$.

- We are interested in modeling $\mu_Y = \pi$:

$$g(\pi) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

Link Function for Logistic Regression

Because π is bounded by 0 and 1, we cannot model it directly—we must apply an appropriate link function.

- Logistic regression uses the *logit link*.
- Given π, we can define the *odds* of success as:

$$O_s = \frac{\pi}{1 - \pi}$$

- Because $\pi \in [0, 1]$, we know that $O_s \geq 0$.
- We take the natural log of the odds as the last step to fully map π to the real line.

$$\text{logit}(\pi) = \ln\left(\frac{\pi}{1 - \pi}\right)$$

Fully Specified Logistic Regression Model

Our final logistic regression model is:

$$Y \sim \text{Bin}(\pi, 1)$$

$$\text{logit}(\pi) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

The fitted model can be represented as:

$$\text{logit}(\hat{\pi}) = \hat{\beta}_0 + \sum_{p=1}^{P} \hat{\beta}_p X_p$$

The fitted coefficients, $\{\hat{\beta}_0, \hat{\beta}_p\}$, are interpreted in units of *log odds*.

Logistic Regression Example

If we fit a logistic regression model to the test-passing data plotted above, we get:

$$\text{logit}(\hat{\pi}_{pass}) = -3.414 + 0.683 X_{study}$$

- A student who does not study at all has -3.414 log odds of passing the exam.
- For each additional hour of study, a student's log odds of passing increase by 0.683 units.

Log odds do not lend themselves to interpretation.

- We can convert the effects back to an odds scale by exponentiation.
- $\hat{\beta}$ has log odds units, but $e^{\hat{\beta}}$ has odds units.

Interpretations

Exponentiating the coefficients also converts the additive effects to multiplicative effects.

- $\ln(AB) = \ln(A) + \ln(B)$
- We can interpret $\hat{\beta}$ as we would in linear regression:
  - A unit change in X_p produces an expected change of $\hat{\beta}_p$ units in $\text{logit}(\pi)$.
- After exponentiation, however, unit changes in X_p imply multiplicative changes in $O_s = \pi/(1-\pi)$.
  - A unit change in X_p results in multiplying O_s by $e^{\hat{\beta}_p}$.

Interpretations

Exponentiating the coefficients in our toy test-passing example produces the following interpretations:

- A student who does not study is expected to pass the exam with odds of 0.033.
- For each additional hour a student studies, their odds of passing increase by 1.98 *times*.
  - Odds of passing are *multiplied* by 1.98 for each extra hour of study.

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  - Odds of passing are *multiplied* by 1.98 for each extra hour of study.

Due to the confusing interpretations of the coefficients, we often focus on the valance of the effects:

- Additional study time is associated with increased odds of passing.
- $\hat{\beta}_p > 0$ = "Increased Success", $e^{\hat{\beta}_p} > 1$ = "Increased Success"

Multiple Logistic Regression

The preceding example was a *simple logistic regression*.

- Including multiple predictor variables in the systematic component leads to *multiple logistic regression*.
- The relative differences between simple logistic regression and multiple logistic regression are the same as those between simple linear regression and multiple linear regression.
  - The only important complication is that the regression coefficients become partial effects.

Multiple Logistic Regression Example

Suppose we want to predict the probability of a patient having "high" blood glucose from their age, BMI, and average blood pressure.

- We could do so with the following model:

$$\text{logit}(\pi_{hi.gluc}) = \beta_0 + \beta_1 X_{age.40} + \beta_2 X_{BMI.25} + \beta_3 X_{BP.100}$$

- By fitting this model to our usual "diabetes" data we get:

$$\text{logit}(\hat{\pi}_{hi.gluc}) = -1.888 + 0.022 X_{age.40} + 0.126 X_{BMI.25} + 0.027 X_{BP.100}$$

- Exponentiating the coefficients produces:

$$\frac{\hat{\pi}_{hi.gluc}}{1 - \hat{\pi}_{hi.gluc}} = 0.151 \times 1.023^{X_{age.40}} \times 1.134^{X_{BMI.25}} \times 1.028^{X_{BP.100}}$$

Exponentiating the Systematic Component

$$\text{logit}(\hat{\pi}_{hi.gluc}) = -1.888 + 0.022X_{age.40} + 0.126X_{BMI.25} + 0.027X_{BP.100}$$

$$e^{\text{logit}(\hat{\pi}_{hi.gluc})} = e^{\left(-1.888 + 0.022X_{age.40} + 0.126X_{BMI.25} + 0.027X_{BP.100}\right)}$$

$$\frac{\hat{\pi}_{hi.gluc}}{1-\hat{\pi}_{hi.gluc}} = e^{-1.888} \times e^{0.022X_{age.40}} \times e^{0.126X_{BMI.25}} \times e^{0.027X_{BP.100}}$$

$$= \left(e^{-1.888}\right) \times \left(e^{0.022}\right)^{X_{age.40}} \times \left(e^{0.126}\right)^{X_{BMI.25}} \times \left(e^{0.027}\right)^{X_{BP.100}}$$

$$= 0.151 \times 1.023^{X_{age.40}} \times 1.134^{X_{BMI.25}} \times 1.028^{X_{BP.100}}$$

Multinomial Logistic Regression

Multi-Class Outcomes

So, what do we do if our outcome takes more than two levels?

- Voting intention = {Will vote, Won't vote, Not sure}
- Preferred caffeine source = {Coffee, Tea, Energy drink, None}
- Current mood = {Happy, Sad, Angry, Neutral}

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We saw that using a nominal variable with L response levels as a predictor requires creating $L - 1$ dummy codes.

- We could solve our problem by estimating $L - 1$ separate logistic regression models.
- Do you see any problems with that approach?

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- We could solve our problem by estimating $L - 1$ separate logistic regression models.
- Do you see any problems with that approach?

We have a better way: *Multinomial logistic regression.*

Defining the Multinomial Logistic Regression Model

In multinomial logistic regression problems, we are modeling multi-class nominal data:

- Usual coding: $Y \in \{1, 2, \ldots, L\}$.

The *Multinomial* distribution—a generalization of the binomial distribution—is a good way to represent this kind of data.

- The systematic component in our multinomial logistic regression model will be the multinomial distribution.

We are interested in modeling the $L - 1$ probabilities, $\pi_l = P(Y = l)$, of endorsing each response level instead of the *baseline* level.

$$g(\pi_l) = \beta_{l0} + \sum_{p=1}^{P} \beta_{lp} X_p, \quad l = 2, 3, \ldots, L$$

Full Multinomial Logistic Regression Model

Given L unique response levels for Y, our final multinomial logistic regression model is:

$$Y \sim \text{Multinom}(\Pi, \mathbf{1}), \quad \Pi = \{\pi_2, \pi_3, \ldots, \pi_L\}$$

$$\text{logit}(\pi_l) = \beta_{l0} + \sum_{p=1}^{P} \beta_{lp} X_p, \quad l = 2, 3, \ldots, L$$

The fitted model can be represented as:

$$\text{logit}(\hat{\pi}_l) = \hat{\beta}_{l0} + \sum_{p=1}^{P} \hat{\beta}_{lp} X_p, \quad l = 2, 3, \ldots, L$$

Note that we, *simultaneously*, estimate $L - 1$ separate sets of coefficients, $\{\beta_{l0}, \beta_{lp}\}$.

Example

Suppose we want to predict the probability of a patient having "high" or "moderate" blood glucose, versus "low" blood glucose, from their age, BMI, and average blood pressure.

- We could do so with the following model:

$$\text{logit}(\pi_l) = \beta_{l0} + \beta_{l1} X_{age.40} + \beta_{l2} X_{BMI.25} + \beta_{l3} X_{BP.100}$$

- By fitting this model to our usual "diabetes" data we get:

$$\text{logit}(\hat{\pi}_{hi.gluc}) = -0.022 + 0.035 X_{age.40} + 0.241 X_{BMI.25} + 0.067 X_{BP.100}$$

$$\text{logit}(\hat{\pi}_{mid.gluc}) = 1.626 + 0.016 X_{age.40} + 0.132 X_{BMI.25} + 0.046 X_{BP.100}$$

Example

- Exponentiating the coefficients produces:

$$\frac{\hat{\pi}_{hi.gluc}}{\hat{\pi}_{low.gluc}} = 0.978 \times 1.036^{X_{age.40}} \times 1.272^{X_{BMI.25}} \times 1.07^{X_{BP.100}}$$

$$\frac{\hat{\pi}_{mid.gluc}}{\hat{\pi}_{low.gluc}} = 5.084 \times 1.016^{X_{age.40}} \times 1.141^{X_{BMI.25}} \times 1.047^{X_{BP.100}}$$

Classification

Predictions from Logistic Regression

Given a fitted logistic regression model, we can get predictions for new observations of $\{X_p\}$, $\{X'_p\}$.

- Directly applying $\{\hat{\beta}_0, \hat{\beta}_p\}$ to $\{X'_p\}$ will produce predictions on the scale of η:

$$\hat{\eta}' = \hat{\beta}_0 + \sum_{p=1}^{P} \hat{\beta}_p X'_p$$

- By applying the inverse link function, $g^{-1}(\cdot)$, to $\hat{\eta}'$, we get predicted success probabilities:

$$\hat{\pi}' = g^{-1}(\hat{\eta}')$$

Predictions from Logistic Regression

In logistic regression, the inverse link function, $g^{-1}(\cdot)$, is the *logistic function*:

$$\text{logistic}(X) = \frac{e^X}{1 + e^X}$$

So, we convert $\hat{\eta}'$ to $\hat{\pi}'$ by:

$$\hat{\pi}' = \frac{e^{\hat{\eta}'}}{1 + e^{\hat{\eta}'}} = \frac{\exp\left(\hat{\beta}_0 + \sum_{p=1}^{P} \hat{\beta}_p X'_p\right)}{1 + \exp\left(\hat{\beta}_0 + \sum_{p=1}^{P} \hat{\beta}_p X'_p\right)}$$

Classification with Logistic Regression

Once we have computed the predicted success probabilities, $\hat{\pi}'$, we can use them to classify new observations.

- By choosing a threshold on $\hat{\pi}'$, say $\hat{\pi}' = t$, we can classify the new observations as "Successes" or "Failures":

$$\hat{Y}' = \begin{cases} 1 & if \quad \hat{\pi}' \geq t \\ 0 & if \quad \hat{\pi}' < t \end{cases}$$

Classification Example

Say we want to classify a new patient into either the "high glucose" group or the "not high glucose" group using the model fit above.

- Assume this patient has the following characteristics:
  - They are 57 years old
  - Their BMI is 28
  - Their average blood pressure is 92

First we plug their predictor data into the fitted model to get their model-implied η:

$$\begin{aligned}\hat{\eta} &= -1.888 + 0.022(57 - 40) + 0.126(28 - 25) + 0.027(92 - 100) \\ &= -1.347\end{aligned}$$

Classification Example

Next we convert the predicted η value into a model-implied success probability by applying the logistic function:

$$0.206 = \frac{e^{-1.347}}{1 + e^{-1.347}}$$

Finally, to make the classification, assume a threshold of $\hat{\pi}' = 0.5$ as the decision boundary.

- Because $0.206 < 0.5$ we would classify this patient into the "low glucose" group.

Predictions from Multinomial Logistic Regression

Generating predictions from a multinomial logistic regression model is nearly identical to predicting with a logistic regression model.

- The only difference is that the multinomial logistic regression model will produce L distinct estimates of $\hat{\eta}'_l$ and $\hat{\pi}'_l$:

$$\hat{\eta}'_l = \begin{cases} \hat{\beta}_{l0} + \sum_{p=1}^{P} \hat{\beta}_{lp} X'_p & \text{if } l > 1 \\ 0 & \text{if } l = 1 \end{cases}$$

$$\hat{\pi}'_l = g^{-1}(\hat{\eta}'_l)$$

Predictions from Multinomial Logistic Regression

In multinomial logistic regression, the inverse link function, $g^{-1}(\cdot)$, is the *softmax function*:

$$\text{softmax}(X_l) = \frac{e^{X_l}}{\sum_{j=1}^{J} e^{X_j}}$$

So, we convert each $\hat{\eta}'_l$ to $\hat{\pi}'_l$ by:

$$\hat{\pi}'_l = \frac{e^{\hat{\eta}'_l}}{\sum_{j=1}^{J} e^{\hat{\eta}'_j}} = \begin{cases} \frac{\exp\left(\hat{\beta}_{l0} + \sum_{p=1}^{P} \hat{\beta}_{lp} X'_p\right)}{1 + \sum_{j=2}^{J} \exp\left(\hat{\beta}_{j0} + \sum_{p=1}^{P} \hat{\beta}_{jp} X'_p\right)} & \text{if } l > 1 \\ \frac{1}{1 + \sum_{j=2}^{J} \exp\left(\hat{\beta}_{j0} + \sum_{p=1}^{P} \hat{\beta}_{jp} X'_p\right)} & \text{if } l = 1 \end{cases}$$

Classification with Multinomial Logistic Regression

Once we have computed the L predicted success probabilities, $\hat{\pi}'_l$, we can use them to classify new observations.

- Each observation is labeled with the response level associated with the largest $\hat{\pi}'_l$
- For example:
  - Given the response options $Y \in \{\text{Coffee, Tea, Energy Drinks, None}\}$
  - And corresponding success probabilities $\hat{\pi}_l \in \{0.45, 0.2, 0.15, 0.2\}$
  - We would assign the observation to the "Coffee" group

Classification Example

Let's re-classify our patient into either the "high glucose", "moderate glucose", or "low glucose" group using the model fit above.

- First we plug their predictor data into the fitted model to get their set of model-implied η_l values:

$$\text{logit}\left(\frac{\pi_{low.gluc}}{\pi_{low.gluc}}\right) =$$

$$0 + 0\,(57 - 40) \quad + 0\,(28 - 25) \quad + 0\,(92 - 100) \quad = 0$$

$$\text{logit}\left(\frac{\pi_{mid.gluc}}{\pi_{low.gluc}}\right) =$$

$$1.626 + 0.016\,(57 - 40) + 0.132\,(28 - 25) + 0.046\,(92 - 100) = 1.929$$

$$\text{logit}\left(\frac{\pi_{hi.gluc}}{\pi_{low.gluc}}\right) =$$

$$-0.022 + 0.035\,(57 - 40) + 0.241\,(28 - 25) + 0.067\,(92 - 100) = 0.762$$

Classification Example

- Next we apply the softmax function to convert the predicted η_l values into model-implied success probabilities:

$$\hat{\pi}_{low.gluc} = \frac{1}{1 + e^{1.929} + e^{0.762}} = 0.1$$

$$\hat{\pi}_{mid.gluc} = \frac{e^{1.929}}{1 + e^{1.929} + e^{0.762}} = 0.687$$

$$\hat{\pi}_{hi.gluc} = \frac{e^{0.762}}{1 + e^{1.929} + e^{0.762}} = 0.214$$

- Finally, to make the classification, we find the largest $\hat{\pi}'_l$:
  - Because $\hat{\pi}_{mid.gluc} = 0.687$ is the largest, we would classify this patient into the "moderate glucose" group.

Classification Error

The MSE is not an appropriate error measure for classification.

- The differences between predicted and observed outcomes have little meaning.

One of the most popular error measures is the *Cross-Entropy Error*:

$$CEE = -N^{-1} \sum_{n=1}^{N} Y_n \ln(\hat{\pi}_n) + (1 - Y_n) \ln(1 - \hat{\pi}_n)$$

$$CEE = -N^{-1} \sum_{n=1}^{N} \sum_{l=1}^{L} \mathbf{I}(Y_n = l) \ln(\hat{\pi}_{nl})$$

- The CEE is sensitive to classification confidence.
- Stronger predictions are more heavily weighted.

Why not Missclassification Rate?

The missclassification rate is a naïvely appealing option.

- The proportion of cases assigned to the wrong group

Consider two perfect classifiers:

1. $P(\hat{Y}_n = 1 | Y_n = 1) = 0.90$, $P(\hat{Y}_n = 1 | Y_n = 0) = 0.10$, $n = 1, 2, \ldots, N$
2. $P(\hat{Y}_n = 1 | Y_n = 1) = 0.55$, $P(\hat{Y}_n = 1 | Y_n = 0) = 0.45$, $n = 1, 2, \ldots, N$

Both of these classifiers will have the same missclassification rate.

- Neither model ever makes an incorrect group assignment.

The first model will have a lower CEE.

- The classifications are made with higher confidence.
- $CEE_1 = 0.105$, $CEE_2 = 0.598$

Conclusion

- The Generalized Linear Model is a flexible class of models that we can use for non-normally distributed outcomes.
  - Multiple linear regression is a special type of GLM.
- We cannot model nominal outcomes with linear regression.
  - We should use some form of logistic regression.
- We use logistic regression for binary outcomes and multinomial logistic regression for multi-class nominal outcomes.
- We must take care when interpreting the coefficients from logistic regression models.
- We can use the estimated success probabilities from a fitted model to classify new observations.