Generalized Linear Model & Logistic Regression

Fundamental Techniques in Data Science

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Outline

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

Extending the General 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 ⊂ 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

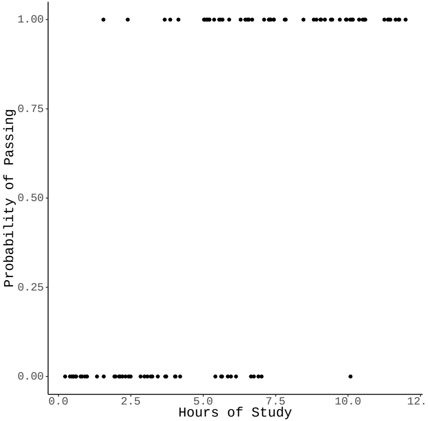
We want to build a model that predicts class membership based on some set of interesting features.

- 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.

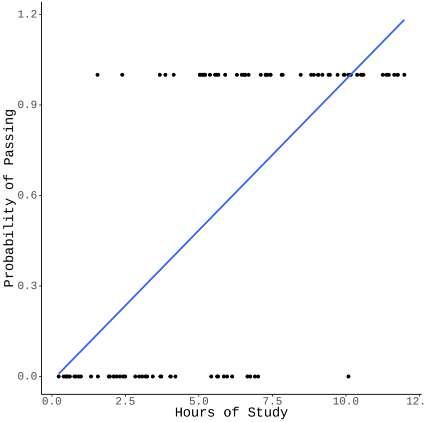
- The probability of passing must be between 0 and 1.
- We care about the probability of passing, but we only observe absolute success or failure.
  - $Y \in \{1, 0\}$



Linear Regression for Binary Outcomes?

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

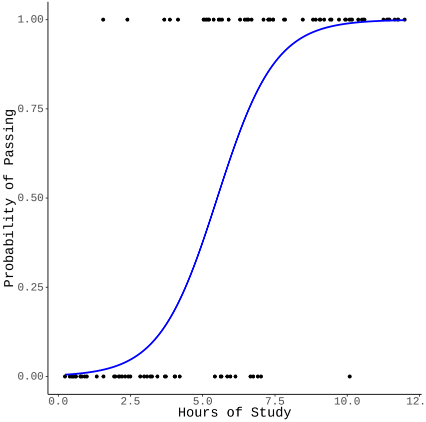
- Hmm...notice any problems?



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:

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

- 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

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

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

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

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

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

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:

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

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.

Evaluating Classification Performance

Confusion Matrix

One of the most direct ways to evaluate classification performance is to tabulate the true and predicted classes.

- Such a cross-tabulation is called a *confusion matrix*.

	Predicted	
True	Low	High
Low	348	9
High	78	7

Confusion Matrix of Blood Glucose Level

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	Predicted	
True	Low	High
Low	348	9
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Confusion Matrix of Blood Glucose Level

We can summarize the confusion matrix in many ways.

- Different summaries highlight different aspects of the classifier's performance.

Summarizing the Confusion Matrix

Sensitivity (Recall, Hit Rate, True-Positive Rate):

$$Sensitivity = \frac{True\ Postives}{True\ Positives + False\ Negatives} = \frac{True\ Postives}{Total\ Positives}$$

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Summarizing the Confusion Matrix

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Specificity (Selectivity, True-Negative Rate):

$$Specificity = \frac{True\ Negatives}{True\ Negatives + False\ Positives} = \frac{True\ Negatives}{Total\ Negatives}$$

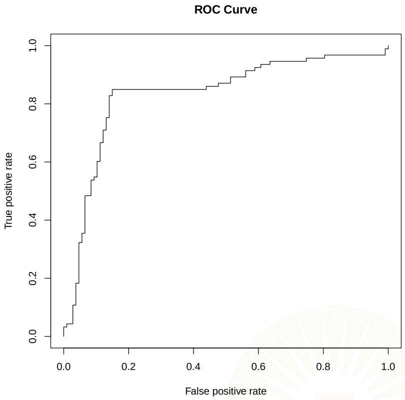
Accuracy:

$$Accuracy = \frac{True\ Positives + True\ Negatives}{TP + TN + FP + FN} = \frac{Correct\ Classifications}{Total\ Cases}$$

ROC Curve

We can visualize the classification performance via a *Reciever-Operator Characteristic* (ROC) Curve.

- Y-Axis: Sensitivity
- X-Axis: 1-Specificity



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*:

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

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

Why not Accuracy?

The accuracy is a naïvely appealing option.

- The proportion of cases assigned to the correct group

Consider two perfect classifiers:

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

Both of these classifiers will have the same accuracy.

- 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.