Lecture 18: Multiclass Logistic Regression

CS109A Introduction to Data Science
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Lecture Outline: Multiclass Classification

Multinomial Logistic Regression
OvR Logistic Regression
$k$-NN for multiclass
Logistic Regression for predicting 3+ Classes

There are several extensions to standard logistic regression when the response variable $Y$ has more than 2 categories. The two most common are:

1. **Ordinal logistic regression**
2. **Multinomial logistic regression.**

Ordinal logistic regression is used when the categories have a specific hierarchy (like class year: Freshman, Sophomore, Junior, Senior; or a 7-point rating scale from strongly disagree to strongly agree).

Multinomial logistic regression is used when the categories have no inherent order (like eye color: blue, green, brown, hazel, et...).
Multinomial Logistic Regression
Multinomial Logistic Regression

There are two common approaches to estimating a nominal (not-ordinal) categorical variable that has more than 2 classes. The first approach sets one of the categories in the response variable as the reference group, and then fits separate logistic regression models to predict the other cases based off of the reference group. For example, we could attempt to predict a student’s concentration:

\[
y = \begin{cases} 
1 & \text{if Computer Science (CS)} \\
2 & \text{if Statistics} \\
3 & \text{otherwise}
\end{cases}
\]

from predictors $X_1$ number of psets per week, $X_2$ how much time playing video games per week, etc.
Multinomial Logistic Regression (cont.)

We could select the $y = 3$ case as the reference group (other concentration), and then fit two separate models: a model to predict $y = 1$ (CS) from $y = 3$ (others) and a separate model to predict $y = 2$ (Stat) from $y = 3$ (others).

Ignoring interactions, how many parameters would need to be estimated? $p + 1$ coefficients for each model: $p = \# \text{predictors}$

$K - 1$ models: $K$ # classes in $y$

How could these models be used to estimate the probability of an individual falling in each concentration?
Multinomial Logistic Regression: the model

To predict $K$ classes ($K > 2$) from a set of predictors $X$, a multinomial logistic regression can be fit:

\[
\ln \left( \frac{P(Y = 1)}{P(Y = K)} \right) = \beta_{0,1} + \beta_{1,1}X_1 + \beta_{2,1}X_2 + \cdots + \beta_{p,1}X_p
\]
\[
\ln \left( \frac{P(Y = 2)}{P(Y = K)} \right) = \beta_{0,2} + \beta_{1,2}X_1 + \beta_{2,2}X_2 + \cdots + \beta_{p,2}X_p
\]
\[
\vdots
\]
\[
\ln \left( \frac{P(Y = K - 1)}{P(Y = K)} \right) = \beta_{0,K-1} + \beta_{1,K-1}X_1 + \beta_{2,K-1}X_2 + \cdots + \beta_{p,K-1}X_p
\]

Each separate model can be fit as independent standard logistic regression models!
Multinomial Logistic Regression in sklearn

```python
mlogit = LogisticRegression(penalty='none',
    multi_class='multinomial')
mlogit.fit(nfl_19[['ydstogo','down']],nfl_19['playtype'])
print(mlogit.intercept_)
print(mlogit.coef_)
```

```
[[-6.78443446  4.46327069  2.32116377]
 [ 0.08130727  1.86026457]
[-0.10687815  1.33128781]
 [ 0.02557089 -0.52897676]]
```

But wait Kevin, I thought you said we only fit $K - 1$ logistic regression models!?!? Why are there $K$ intercepts and $K$ sets of coefficients??
What is sklearn doing?

The $K - 1$ models in multinomial regression lead to the following probability predictions:

\[
\ln \left( \frac{P(Y = k)}{P(Y = K)} \right) = \beta_{0,k} + \beta_{1,k}X_1 + \beta_{2,k}X_k + \cdots + \beta_{p,k}X_p
\]

This gives us $K - 1$ equations to estimate $K$ probabilities for everyone. But probabilities add up to 1 😊, so we are all set.

Sklearn then converts the above probabilities back into new betas (just like logistic regression, but the betas won’t match):

\[
\ln \left( \frac{P(Y = k)}{P(Y \neq k)} \right) = \beta'_0,k + \beta'_{1,k}X_1 + \beta'_{2,k}X_k + \cdots + \beta'_{p,k}X_p
\]
One vs. Rest (OvR) Logistic Regression

K separate logistic models
One vs. Rest (OvR) Logistic Regression

An alternative multiclass logistic regression model in sklearn is called the ’One vs. Rest’ approach, which is our second method.

If there are 3 classes, then 3 separate logistic regressions are fit, where the probability of each category is predicted over the rest of the categories combined. So for the concentration example, 3 models would be fit:

- a first model would be fit to predict CS from (Stat and Others) combined.
- a second model would be fit to predict Stat from (CS and Others) combined.
- a third model would be fit to predict Others from (CS and Stat) combined.

An example to predict play call from the NFL data follows...
One vs. Rest (OvR) Logistic Regression: the model

To predict $K$ classes ($K > 2$) from a set of predictors $X$, a multinomial logistic regression can be fit:

\[
\ln \left( \frac{P(Y = 1)}{P(Y \neq 1)} \right) = \beta_{0,1} + \beta_{1,1}X_1 + \beta_{2,1}X_2 + \cdots + \beta_{p,1}X_p \\
\ln \left( \frac{P(Y = 2)}{P(Y \neq 2)} \right) = \beta_{0,2} + \beta_{1,2}X_1 + \beta_{2,2}X_2 + \cdots + \beta_{p,2}X_p \\
\vdots \\
\ln \left( \frac{P(Y = K)}{P(Y \neq K)} \right) = \beta_{0,K} + \beta_{1,K}X_1 + \beta_{2,K}X_2 + \cdots + \beta_{p,K}X_p
\]

Again, each separate model can be fit as independent standard logistic regression models!
So how do we convert a set of probability estimates from separate models to one set of probability estimates? The **softmax** function is used. That is, the weights are just normalized for each predicted probability. AKA, predict the 3 class probabilities from each of the 3 models, and just rescale so they add up to 1.

Mathematically that is:

\[
P(y = k | \hat{x}) = \frac{e^{\hat{x}^T \hat{\beta}_k}}{\sum_{j=1}^{K} e^{\hat{x}^T \hat{\beta}_j}}
\]

where \(\hat{x}\) is the vector of predictors for that observation and \(\hat{\beta}_k\) are the associated logistic regression coefficient estimates.
OVR Logistic Regression in Python

```python
ovrlogit = LogisticRegression(penalty='none', multi_class='ovr')

ovrlogit.fit(nfl_19[['ydstogo','down']],nfl_19['playtype'])
print(ovrlogit.intercept_)
print(ovrlogit.coef_)
```

```
[-10.03308293  2.47802369  -0.10976034]
[[ 0.07547391  2.55126265]
 [-0.14272983 -0.98841346]
 [ 0.03672441 -0.03755844]]
```

Phew! This one is as expected 😊
Predicting Type of Play in the NFL

Multinomial Logistic Regression: Predicted Probabilities on 2nd Down

OvR Logistic Regression: Predicted Probabilities on 2nd Down

$X=4$

$X=3$
Classification for more than 2 Categories

When there are more than 2 categories in the response variable, then there is no guarantee that $P(Y = k) \geq 0.5$ for any one category. So any classifier based on logistic regression (or other classification model) will instead have to select the group with the largest estimated probability.

The classification boundaries are then much more difficult to determine mathematically. We will not get into the algorithm for determining these in this class, but we can rely on `predict` and `predict_proba`!
Prediction using Multiclass Logistic Regression

```python
print(mlogit.predict_proba(nfl_19[['ydstogo', 'down']])[0:5,:])
print(mlogit.predict(nfl_19[['ydstogo', 'down']])[0:5])
[[0.001048 0.50329827 0.49565372]
 [0.01559789 0.30793278 0.67646934]
 [0.17275682 0.14020122 0.68704196]
 [0.82376365 0.00418569 0.17205066]
 [0.001048 0.50329827 0.49565372]]
[1 2 2 0 1]
```

```python
print(ovrlogit.predict_proba(nfl_19[['ydstogo', 'down']])[0:5,:])
print(ovrlogit.predict(nfl_19[['ydstogo', 'down']])[0:5])
[[0.00111671 0.48115571 0.51772757]
 [0.01792012 0.33603242 0.64604746]
 [0.19847963 0.15493954 0.64658083]
 [0.57254676 0.0088239  0.41862935]
 [0.00111671 0.48115571 0.51772757]]
[2 2 2 0 2]
```
Classification Boundary for 3+ Classes in sklearn

It's not easy to do mathematically.
Estimation and Regularization in multiclass settings

There is no difference in the approach to estimating the coefficients in the multiclass setting: we maximize the log-likelihood (or minimize negative log-likelihood).

This combined negative log-likelihood of all $K$ classes is sometimes called the **binary crossentropy**:

$$
\ell = \frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} 1(y_i = k) \ln(\hat{P}(y_i = k)) + 1(y_i \neq k) \ln(1 - \hat{P}(y_i = k))
$$

And regularization can be done like always: add on a penalty term to this loss function based on L1 (sum of the absolute values) or L2 (sum of squares) norms.
Multiclass $k$-NN
Extending the $k$-NN classification model to 3+ classes is much simpler!

Remember, $k$-NN is done in two steps:

1. **Find you $k$ neighbors**: this is still done in the exact same way
   - be careful of the scaling of your predictors!

2. **Predict based on your neighborhood**:
   - Predicting probabilities: just use the observed proportions
   - Predicting classes: plurality wins!
$k$-NN for 3+ Classes: NFL Data

$k = 5$

$k = 20$

$k = 100$

"complex? overfit"

"simpler and "better" for validation set"

"20% sample"
Exercise Time!

Ex. 1 (graded): Basic multiclass Logistic Regression and k-NN in sklearn (15+ min)

Ex. 2 (not graded): A little more thinking and understanding (30+ min)