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. ("nominal" classes)

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...).

we focus on "nominal"

Multinomial Logistic Regression

Multinomial Logistic Regression

OvR

$$\ln\left(\frac{P(Y_i=1)}{P(Y_i\neq 1)}\right)=\beta_0+\beta_1X_1$$

3 of these

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:

(2 models)

Multinomial

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

$$\ln\left(\frac{P(Y_i=1)}{P(Y_i=3)}\right)=\beta_0+\beta_1X_1$$

2 of these

$$\ln\left(\frac{P(Y_i=2)}{P(Y_i=3)}\right)=\beta_2+\beta_3X_1$$

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 $\boxed{y = 3 \text{ case}}$ 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 = #predictors

K−1 models : K=# classes in Y

$(K-1)\cdot(p+1)$

How could these models be used to estimate the probability of an individual falling in each concentration?

Multinomial Logistic Regression: the model ← now the default in multiclass in sklearn

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

(p+1)-Betas

K-1 models

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

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

$$\vdots$$

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

Each separate model can be fit as independent standard logistic regression models!

Multinomial Logistic Regression in sklearn

```
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]]
```

```
pd.crosstab(nfl_19["play_type"],
            nfl_19["playtype"])
```

playtype	0	1	2
play_type			
field_goal	978	0	0
pass	0	0	18981
punt	2150	0	0
qb_kneel	393	0	0
qb_spike	72	0	0
run	0	12994	0

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:

just a subset of all classes

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

$$\vdots$$

K-1 equation

$$P(Y=k) = P(Y=K)e^{\beta_{0,k}+\beta_{1,k}X_1+\beta_{2,k}X_k+\cdots+\beta_{p,k}X_p}$$

This give 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.

since they are fit separately, probabilities may not add up to 1

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!

Softmax

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.

"estimated probability"

Mathematically that is:

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

"sum of probabilities"

where $\vec{x}$ is the vector of predictors for that observation and $\hat{\vec{\beta}}_k$ are the associated logistic regression coefficient estimates.

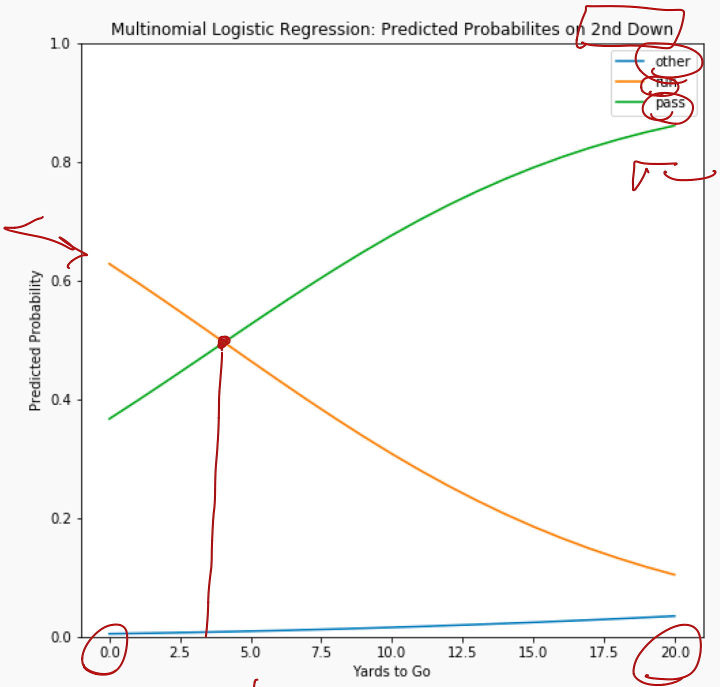
OVR Logistic Regression in Python

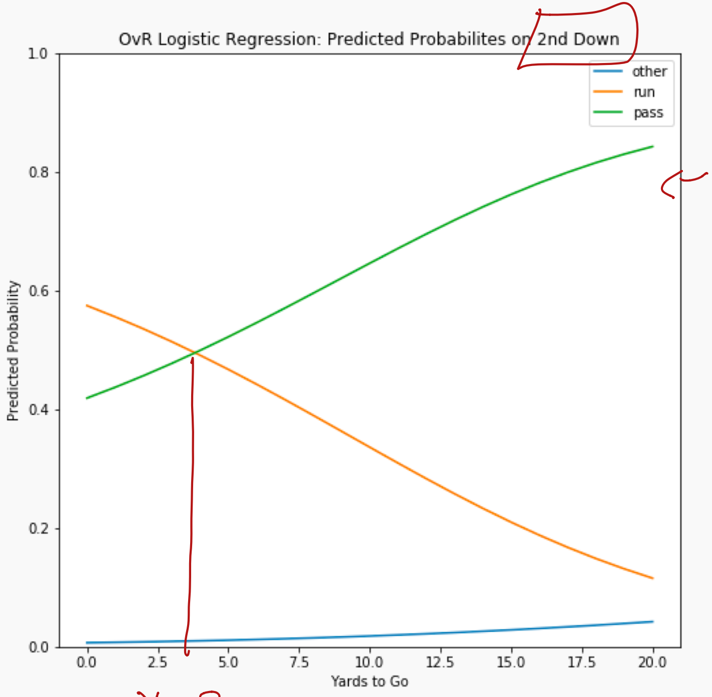
```
ovrlogit = LogisticRegression(penalty='none', multi_class='ovr')

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





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

```
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]
```

$\hat{p}$

$\hat{y}$

1st and 10

```
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]
```

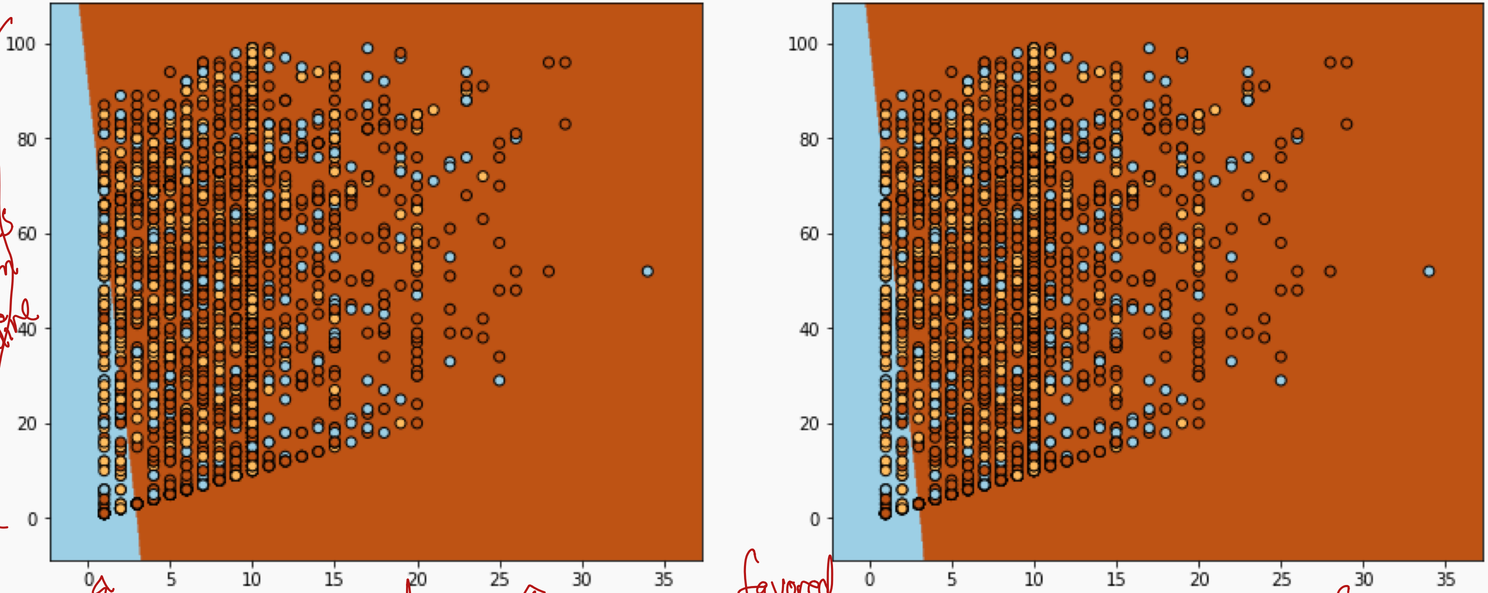
$\hat{p}$

$\hat{y}$

Classification Boundary for 3+ Classes in sklearn

not easy to do mathematically

yard's from the goalline



blue run-favored

brown: pass-favored

yards to go for 1st down.

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**:

looks a little different
our loss function

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

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

k-NN for 3+ Classes

Extending the *k*-NN classification model to 3+ classes is much simpler!

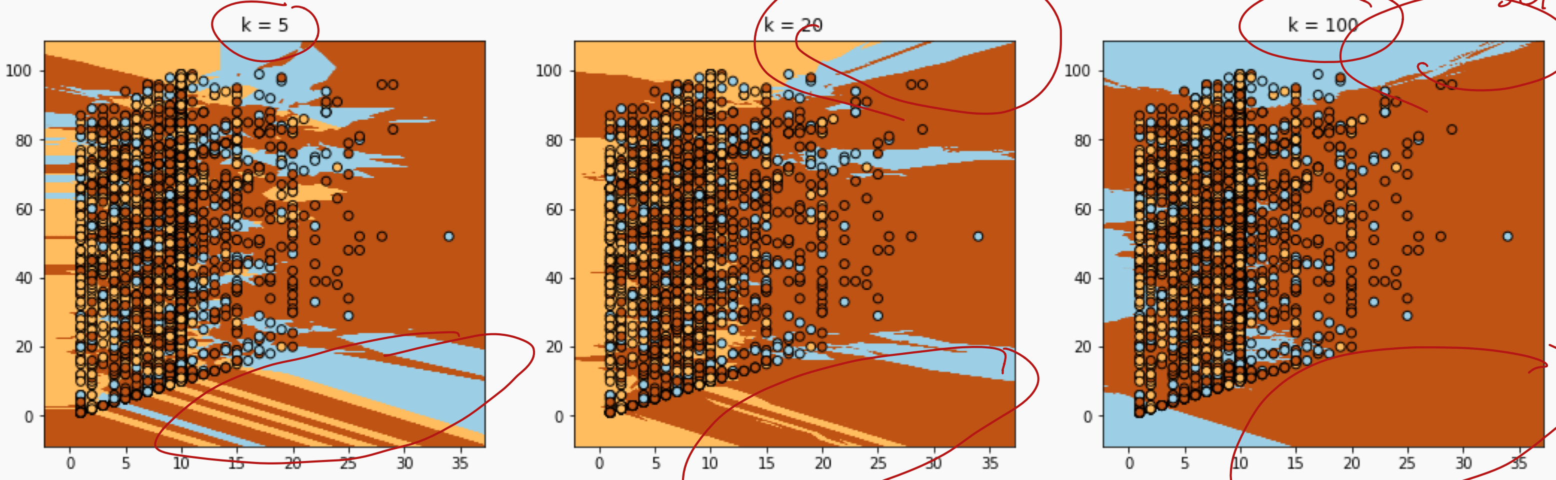
Remember, *k*-NN is done in two steps:

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!

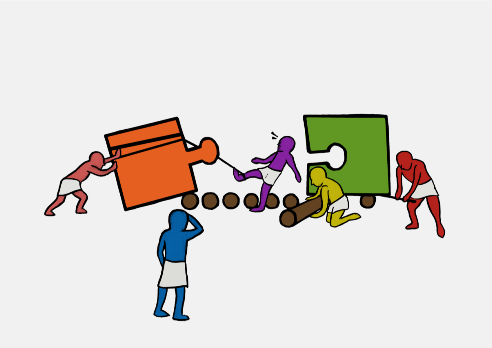
k-NN for 3+ Classes: NFL Data

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)