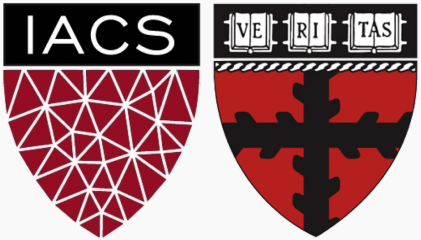
Lecture 18: Multiclass Logistic Regression

CS109A Introduction to Data Science

Pavlos Protopapas, Kevin Rader and Chris Tanner



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:

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

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?

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

```
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]]
```

$\hat{\beta}_0$'s

$\hat{\beta}_1$'s

$\hat{\beta}_2$'s

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

play_type \ playtype	0	1	2
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:

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

$$\vdots$$

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

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):

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

$P(Y\neq k) = 1 - P(Y=k)$

One vs. Rest (OvR) Logistic Regression

K separate models
p+1 parameters.

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!

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.

Mathematically that is:

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

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

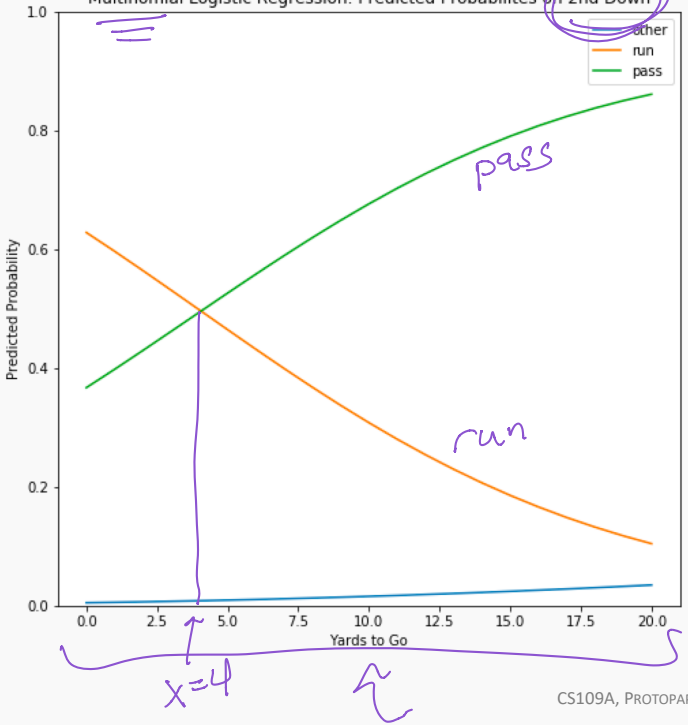
OVR Logistic Regression in Python

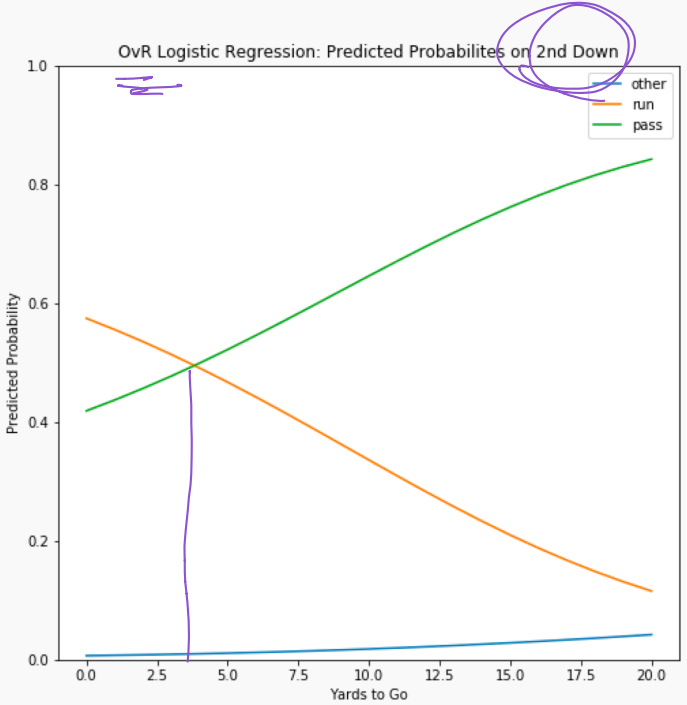
```
ovrlogit = LogisticRegression(penalty='none', multi_class='ovr')

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





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]
```

1st & 10

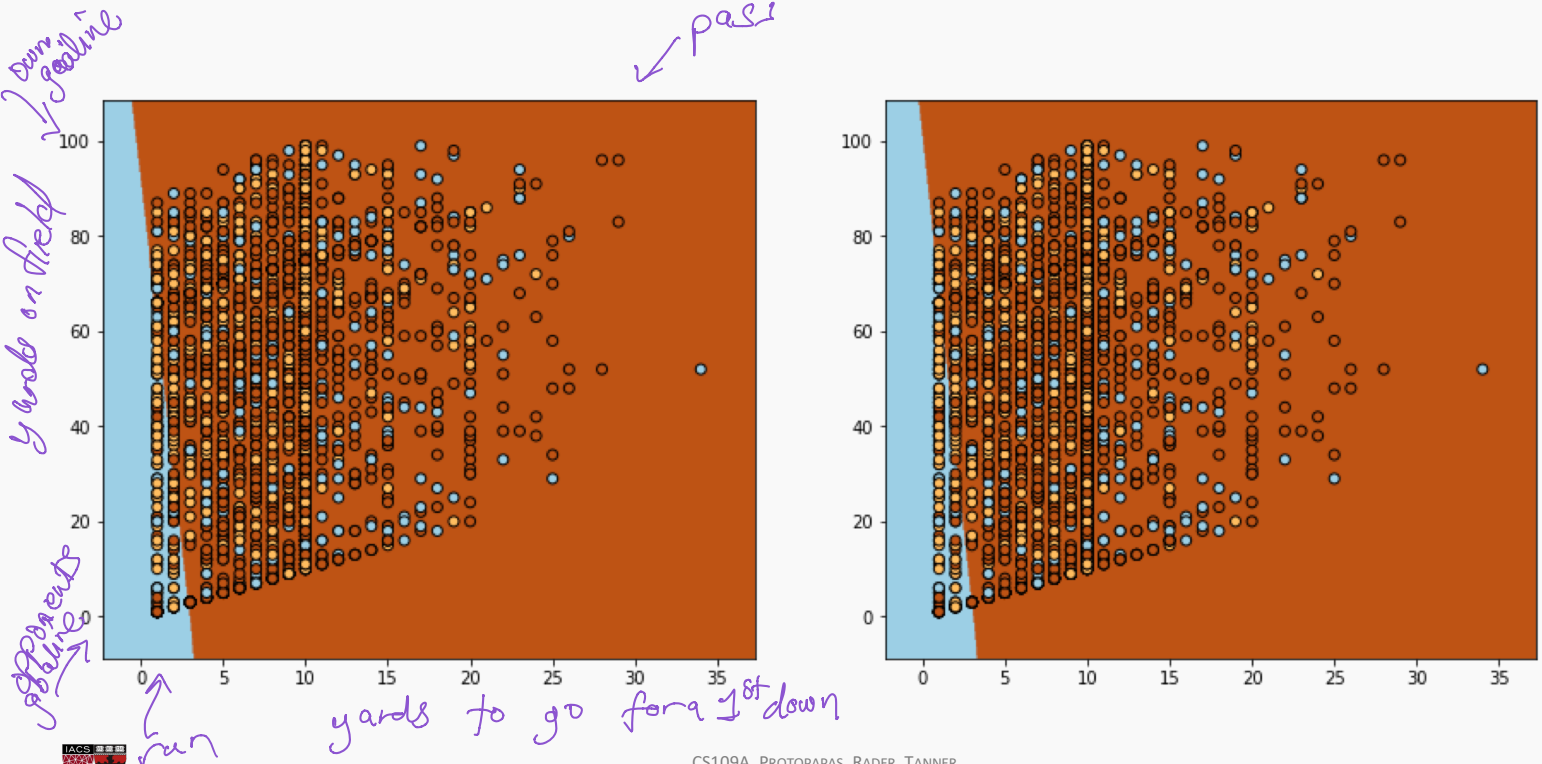
4th

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]
```

Classification Boundary for 3+ Classes in sklearn



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**:

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

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!

no different

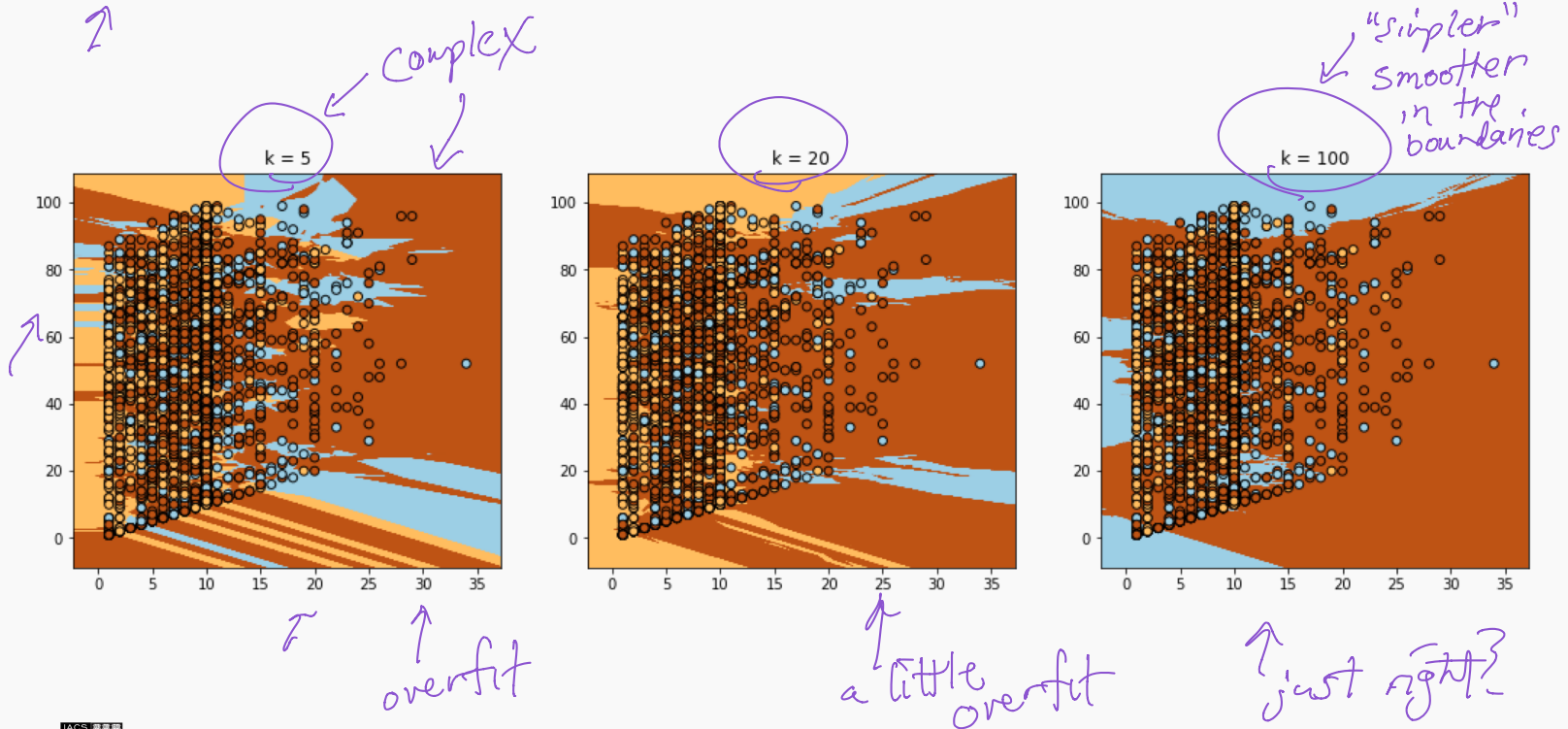
10-NN

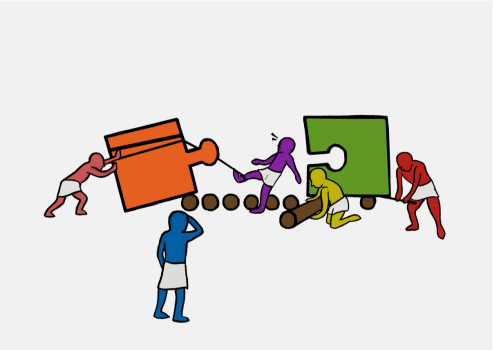
K=10

Class1 Class2 Class3 | K=3 classes

4/10, 2/10, 4/10 → 0.4, 0.2, 0.4

k-NN for 3+ Classes: NFL Data





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)