Elements Of Data Science - F2020

Week 5: Intro to Machine Learning Models

10/12/2020

TODOs

- Readings:
 - Recommended: https://scikit-learn.org/stable/supervised_learning.html
 - Reference: PML Chapter Chap 3
- Answer and submit Quiz 5
- HW1, Due Thurs Oct 22nd, 11:59pm ET

Today

- Multi-Armed Bandit (previous week's slides)
- Intro to Machine Learning Models
 - Various types of ML
 - Linear models

Git Stash

Git will not allow you to pull new version of files if there is a conflict.

Common source of conflict:

- 1. Slide notebook is pushed and pulled
- 2. You make changes to the notebook (encouraged!)
- 3. I post new updates to the notebook (fixes, etc).

Now your version and the current version on github both have new changes: Conflict!

Solution: Stash your changes

```
$ cd eods-f20
$ git stash
$ git pull
```

Questions?

Modeling and ML

- What is a Model?
 - Specification of a mathematical (or probabilistic) relationship between different variables.
- What is Machine Learning?
 - Creating and using models that are learned from data.

Questions for Models

Questions for Models

```
In [2]: df_wine = pd.read_csv('../data/wine_dataset.csv', usecols=['alcohol', 'ash', 'proline', 'hue', 'class'])

Out[2]:

| alcohol | ash | hue | proline | class | |
| 161 | 13.69 | 2.54 | 0.96 | 680.0 | 2 |
| 117 | 12.42 | 2.19 | 1.06 | 345.0 | 1 |
| 19 | 13.64 | 2.56 | 0.96 | 845.0 | 0 |
| 69 | 12.21 | 1.75 | 1.28 | 718.0 | 1 |
| 53 | 13.77 | 2.68 | 1.13 | 1375.0 | 0
```

Questions for Models

```
In [2]: df_wine = pd.read_csv('../data/wine_dataset.csv', usecols=['alcohol', 'ash', 'proline', 'hue', 'class'])

Out[2]:

| alcohol | ash | hue | proline | class | |
| 161 | 13.69 | 2.54 | 0.96 | 680.0 | 2 |
| 117 | 12.42 | 2.19 | 1.06 | 345.0 | 1 |
| 19 | 13.64 | 2.56 | 0.96 | 845.0 | 0 |
| 69 | 12.21 | 1.75 | 1.28 | 718.0 | 1 |
| 53 | 13.77 | 2.68 | 1.13 | 1375.0 | 0
```

- Can we predict label "class" from the other columns? (Classification)
- Can we predict target "hue" from the other columns? (Regression)
- What are the important features when predicting "hue"? (Feature Selection)
- Can a model tell us about how the features and target interact? (Interpretation)
- Do the features group together at all? (Clustering)

Data Vocab for ML

Data Vocab for ML



Data Vocab for ML

```
In [3]: df_wine.sample(5,random_state=1)

Out[3]:

| alcohol | ash | hue | proline | class | |
| 161 | 13.69 | 2.54 | 0.96 | 680.0 | 2 |
| 117 | 12.42 | 2.19 | 1.06 | 345.0 | 1 |
| 19 | 13.64 | 2.56 | 0.96 | 845.0 | 0 |
| 69 | 12.21 | 1.75 | 1.28 | 718.0 | 1 |
| 53 | 13.77 | 2.68 | 1.13 | 1375.0 | 0
```

- \bullet X, features, attributes, independent/exogenous/explanatory variables
 - Ex: alcohol, trip_distance, company_industry
- y, target, label, outcome, dependent/endogenous/response variables
 - Ex: class, hue, tip_amount, stock_price
- $f(X) \rightarrow y$, Model that maps features X to target y

- Supervised vs Unsupervised
 - is there a target/label?

- Supervised vs Unsupervised
 - is there a target/label?
- Regression vs Classification
 - is the target numeric or categorical?

- Supervised vs Unsupervised
 - is there a target/label?
- Regression vs Classification
 - is the target numeric or categorical?
- Interpretation vs Prediction
 - generate predictions or understand interactions?

- Supervised vs Unsupervised
 - is there a target/label?
- Regression vs Classification
 - is the target numeric or categorical?
- Interpretation vs Prediction
 - generate predictions or understand interactions?
- Model Family
 - Linear, Tree, Distance, Probability, Neural Net, Ensemble

Supervised vs Unsupervised vs Reinforcement Learning

Is there a target, *y*?

Other Learning Paradigms

Other Learning Paradigms

- Do we have a mix of labeled and unlabeled?
 - Semi-Supervised Learning
 - Can we use structure of unlabeled data along with labeled?

Other Learning Paradigms

- Do we have a mix of labeled and unlabeled?
 - Semi-Supervised Learning
 - Can we use structure of unlabeled data along with labeled?
- Will we continue getting new data?
 - Online Learning
 - Is there an oracle (ground truth) we can consult?
 - Can we select which points to make predictions on?

Supervised Learning: Regression vs Classification

- **Regression** -> predict a numeric value
 - Ex: tip_amount, stock_price, wine_hue

Interpretation vs Prediction

- Do we care more about understanding how XX relates to yy?
 - Ex: What happens to tip size as taxi trip length increases?
 - Ex: What is the relationship between debt and loan default?
- Do we care more about generating predictions?
 - Ex: For a given trip, what will the tip size likely be?
 - Ex: For a given loan, will there be a default?

Model Families for Supervised Learning

- Linear
 - Simple/Multiple Linear Regression
 - Logistic Regression (for Classification)
 - Support Vector Machines
 - Perceptron
- Tree Based
 - Decision Tree
- Distance Based
 - K-Nearest Neighbor

Model Families for Supervised Learning Continued

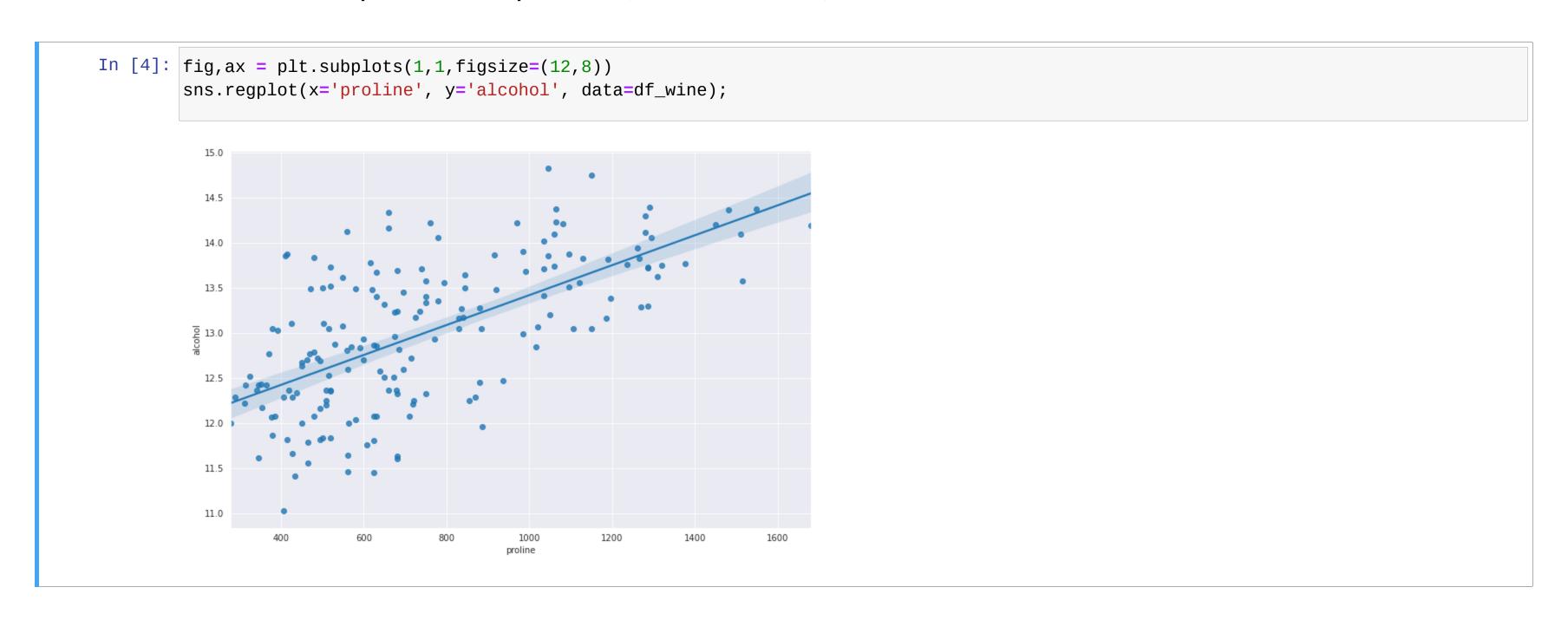
- Probability
 - Naive Bayes?
 - Bayes Net
- Ensemble
 - Random Forest
 - Gradient Boosted Trees
 - Stacking
- Network
 - Multi-layer Perceptron?
 - Deep Neural-Networks/font>
 - Convolutional Neural Nets
 - Recurrant Neural Nets

Example: Regression with a Linear Model

What is the relationship between 'proline' (an amino-acid) and 'alcohol' in wine?

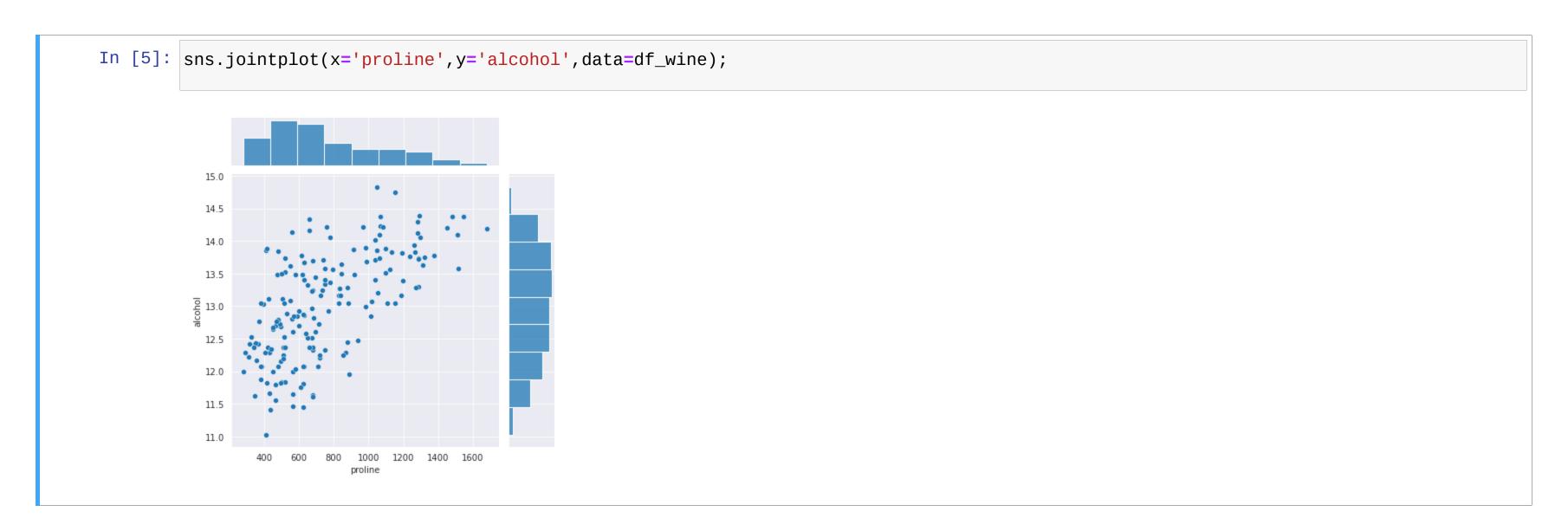
Example: Regression with a Linear Model

What is the relationship between 'proline' (an amino-acid) and 'alcohol' in wine?

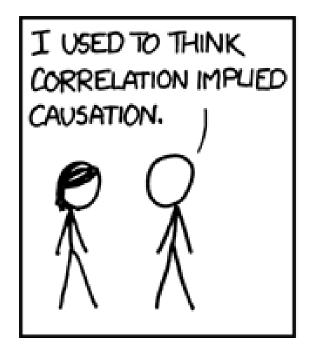


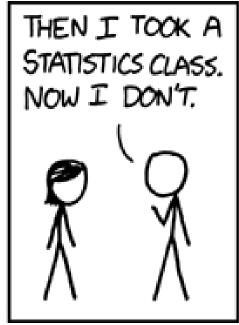
Question: are total_bill and tips correlated?

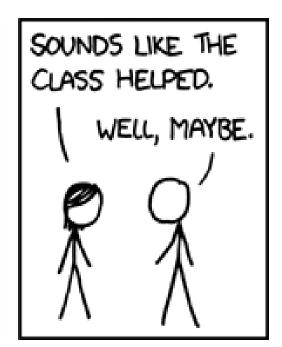
Question: are total_bill and tips correlated?



Obligitory Correlation vs. Causation





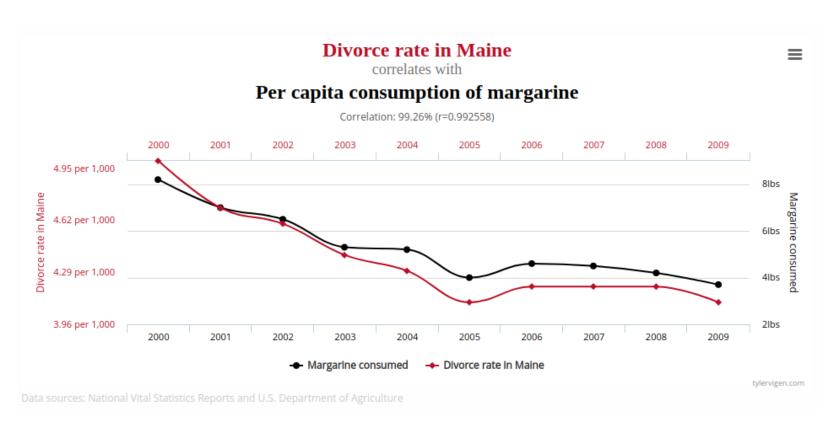


Correlation does not mean causation!

- Causal Inference
 - controlled experiment
 - control for confounding variables

Spurious Correlation

- Also, look hard enough and you'll find correlation.
 - See <u>spurious correlations</u> for examples



- Could calculate Pearson Correlation Coefficient
- Assumes normally distributed data! (which is not true here)
 - On the Effects of Non-Normality on the Distribution of the Sample Product-Moment
 Correlation Coefficient

- Could calculate Pearson Correlation Coefficient
- Assumes normally distributed data! (which is not true here)
 - On the Effects of Non-Normality on the Distribution of the Sample Product-Moment
 Correlation Coefficient

```
In [6]: from scipy.stats import pearsonr
r,p = pearsonr(df_wine.proline,df_wine.alcohol)
print(f'r: {r:.2f}, p: {p:.2f}')
r: 0.64, p: 0.00
```

- Could calculate Pearson Correlation Coefficient
- Assumes normally distributed data! (which is not true here)
 - On the Effects of Non-Normality on the Distribution of the Sample Product-Moment
 Correlation Coefficient

```
In [6]: from scipy.stats import pearsonr
r,p = pearsonr(df_wine.proline,df_wine.alcohol)
print(f'r: {r:.2f}, p: {p:.2f}')
r: 0.64, p: 0.00
```

• We know that as proline goes up alcohol goes up, but by how much?

Python Modeling Libraries

Prediction - scikit-learn



Interpretation - scikit-learn and statsmodels



Additional Tools - mlxtend



Aside: MLxtend and conda-forge

• MLxtend: (machine learning extensions) is a Python library of useful tools for the day-to-day data science tasks.



• Conda-Forge: A community-led collection of recipes, build infrastructure and distributions for the conda package manager.



\$ conda install --name eods-f20 --channel conda-forge mlxtend

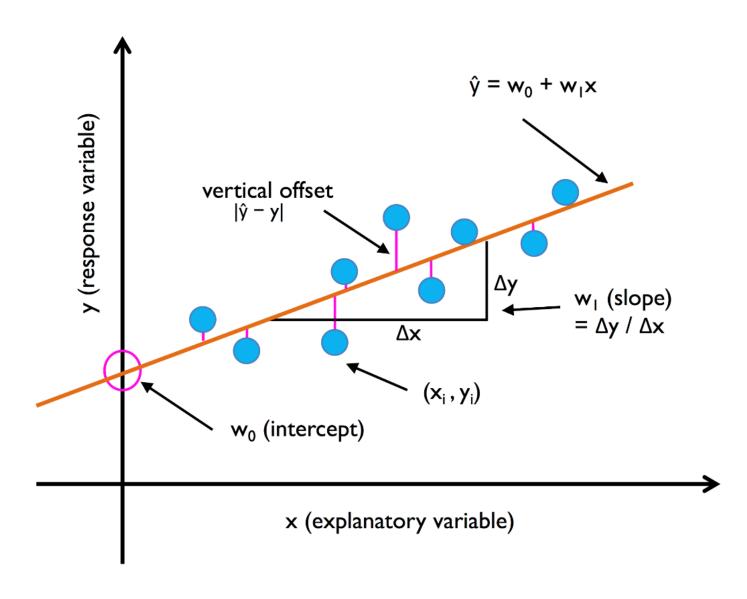
Simple Linear Regression

Simple Linear Regression

$$y = w_1 x + w_0 + \varepsilon_i$$

- y: dependent, endogenous, response, target, label (Ex: alcohol)
- x_i : independent, exogenous, explanatory, feature, attribute (Ex: proline)
- w_1 : coefficient, slope
- w_0 : bias term, intercept
- ε_i : error, hopefully small, often assumed $\mathcal{N}(0,1)$
- Want to find values for w_1 and w_0 that best fit the data.
- Find a line as close to our observations as possible

Simple Linear Regression



from PML

Finding w_1 and w_0 with Ordinary Least Squares

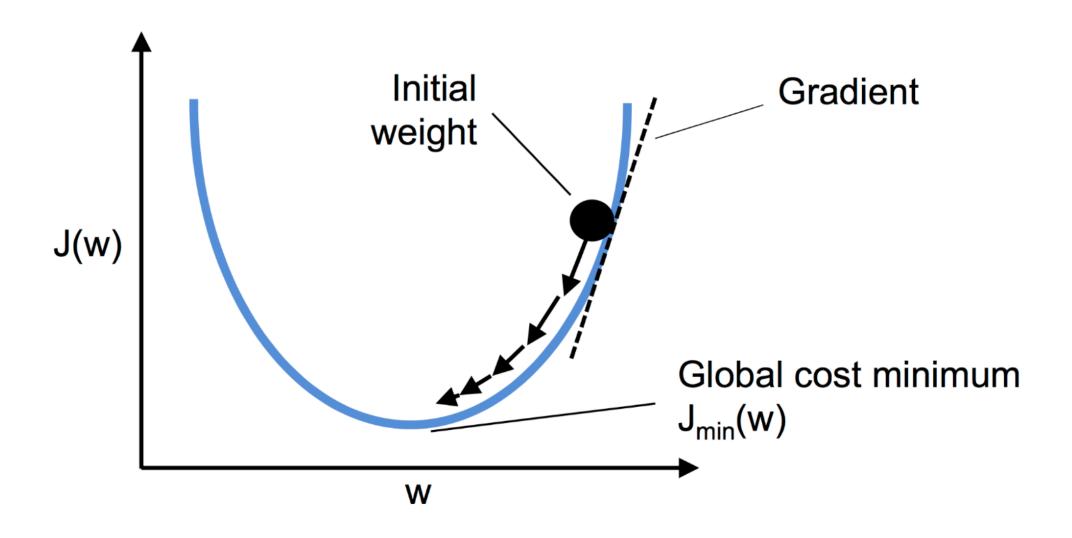
- prediction: $\hat{y}_i = f(x_i) = w_1 x_i + w_0$ error: $error(y_i, \hat{y}_i) = y_i \hat{y}_i$
- sum of squared errors: $\sum_{i=1:n} (y_i \hat{y}_i)^2$
- least squares: make the sum of squared errors as small as possible
- gradient descent: minimize error by following the gradient wrt w_1, w_0
 - can sometime be optimized in closed form
 - often done iteratively

Aside: Gradient Descent

• Want to maximize or minimize something (Ex: squared error)

- **Gradient**: direction, vector of partial derivatives
 - can get complicated, often estimated
- Gradient Descent: take steps wrt the direction of the gradient
 - maximize: in the direction of the gradient
 - minimize: in the opposite direction of the gradient
- Global Maximum/Minimum: the single best solution
- Local Maximum/Minimum: the best solution in the neighborhood

Aside: Gradient Descent Cont.



```
In [7]: # import the model from sklearn
from sklearn.linear_model import LinearRegression
```

```
In [7]: # import the model from sklearn
from sklearn.linear_model import LinearRegression

In [8]: # instantiate the model and set hyperparameters
lr = LinearRegression(fit_intercept=True, # by default
normalize=False) # by default

In [9]: # fit the model
lr.fit(X=df_wine.proline.values.reshape(-1, 1), y=df_wine.alcohol);

In [10]: # display learned coefficients (_ in)
print(lr.coef_)
print(lr.intercept_)

[0.0016595]
11.761148483143147
```

```
In [7]: # import the model from sklearn
         from sklearn.linear_model import LinearRegression
In [8]: # instantiate the model and set hyperparameters
         lr = LinearRegression(fit_intercept=True, # by default
                               normalize=False)
                                                  # by default
In [9]: # fit the model
         lr.fit(X=df_wine.proline.values.reshape(-1, 1), y=df_wine.alcohol);
In [10]: # display learned coefficients (_ in)
         print(lr.coef_)
         print(lr.intercept_)
         [0.0016595]
         11.761148483143147
In [11]: # predict given new values for proline
         X = np.array([1000, 2000]).reshape(-1, 1)
         lr.predict(X)
Out[11]: array([13.42064866, 15.08014884])
```

```
In [12]: df_wine.proline.values[:5]
Out[12]: array([1065., 1050., 1185., 1480., 735.])
```

```
In [12]: df_wine.proline.values[:5]
Out[12]: array([1065., 1050., 1185., 1480., 735.])
In [13]: df_wine.proline.values.shape
Out[13]: (178,)
```

```
In [12]: df_wine.proline.values[:5]
Out[12]: array([1065., 1050., 1185., 1480., 735.])
In [13]: df_wine.proline.values.shape
Out[13]: (178,)
In [14]: df_wine.proline.values.reshape(-1,1).shape
Out[14]: (178, 1)
```

scikit-learn models expect the input features to be 2 dimensional

```
In [12]: df_wine.proline.values[:5]
Out[12]: array([1065., 1050., 1185., 1480., 735.])
In [13]: df_wine.proline.values.shape
Out[13]: (178,)
In [14]: df_wine.proline.values.reshape(-1,1).shape
Out[14]: (178, 1)
```

-1 means "infer from the data"

```
In [15]: print(f'beta={lr.coef_[0]:0.3f}, alpha={lr.intercept_:0.3f}')
beta=0.002, alpha=11.761
```

```
In [15]: print(f'beta={lr.coef_[0]:0.3f}, alpha={lr.intercept_:0.3f}')
    beta=0.002, alpha=11.761

In [16]: print(f'alchohol = {lr.coef_[0]:0.3f}*proline + {lr.intercept_:0.3f}')
    alchohol = 0.002*proline + 11.761
```

- When proline goes up by 1, alcohol goes up by .002
- When proline is 0, alcohol is 11.761

Plotting The Model

Plotting The Model

```
In [17]: x_predict = [df_wine.proline.min(),df_wine.proline.max()]
          y_hat = lr.predict(np.array(x_predict).reshape(-1,1))
          fig,ax = plt.subplots(1,1,figsize=(12,8))
          ax = sns.scatterplot(x=df_wine.proline,y=df_wine.alcohol);
          ax.plot(x_predict,y_hat);
             15.0
            14.5
             14.0
             13.5
           을 13.0
            12.5
             12.0
             11.5
            11.0
                      400
                                              1000
                                                              1400
                                                                      1600
                                             proline
```

Multiple Linear Regression

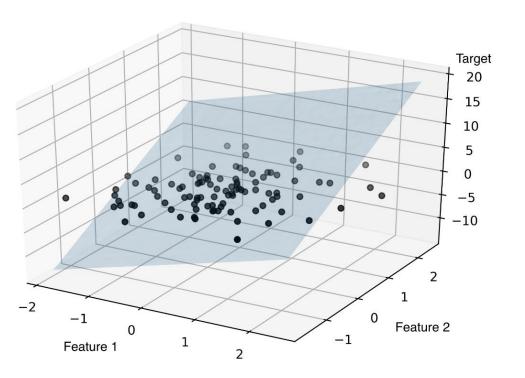
• Including multiple independent variables

$$y_i = w_0 + w_1 x_{i1} + w_2 x_{i2} + \dots + w_m x_{im} + \varepsilon_i$$

Ex:

alcohol =
$$w_0 + w_1^*$$
proline + w_2^* hue

Objective: Find a plane that falls as close to our points as possible



Multiple Linear Regression in scikit-learn

Multiple Linear Regression in scikit-learn

```
In [18]: mlr = LinearRegression()
    mlr.fit(df_wine[['proline','hue']], y=df_wine.alcohol);

for (name,coef) in zip(['proline','hue'],mlr.coef_):
        print(f'{name:10s} : {coef: 0.3f}')
    print(f'{"intercept":10s} : {mlr.intercept_:0.3f}')

proline : 0.002
    hue : -0.842
    intercept : 12.459
```

- If we hold everything else constant, what effect does the variable have
- If hue is held constant, a rise of 1 proline -> rise of .002 in alcohol
- If proline is held constant, a rise of 1 hue -> decrease of .842 in alcohol
- Can add interaction terms to allow both to move
 - Ex: hue * proline
 - more complicated to interpret

Multiple Linear Regression in statsmodels

Multiple Linear Regression in statsmodels

```
In [19]: import statsmodels.api as sm
           X = df_wine[['proline', 'hue']]
           X = sm.add\_constant(X)
           y = df_wine.alcohol
           sm_mlr = sm.OLS(y,X).fit() # Note: X,y passed as parameters to object, not fit
           sm_mlr.summary()
Out[19]:
           OLS Regression Results
            Dep. Variable:
                            alcohol
                                            R-squared:
                                                            0.467
            Model:
                            OLS
                                            Adj. R-squared:
                                                            0.461
                                                           76.79
                                            F-statistic:
            Method:
                            Least Squares
                            Mon, 19 Oct 2020 Prob (F-statistic): 1.15e-24
            Date:
                                            Log-Likelihood:
                                                            -158.89
            Time:
                            17:42:49
            No. Observations: 178
                                                            323.8
                                            AIC:
                                                            333.3
                                            BIC:
            Df Residuals:
                            175
                            2
            Df Model:
            Covariance Type:
                            nonrobust
                                                [0.025
                                                       0.975]
                    coef
                            std err t
                                          P>|t|
                                   61.347
                                          0.000 12.058 12.860
                    12.4593 0.203
            const
            proline 0.0018
                            0.000
                                   12.325 0.000 0.002
                                                        0.002
                    -0.8418 0.202
                                  -4.175 0.000 -1.240
                                                        -0.444
```

Omnibus:	0.751	Durbin-Watson:	1.734
Prob(Omnibus):	0.687	Jarque-Bera (JB):	0.606
Skew:	0.142	Prob(JB):	0.739
Kurtosis:	3.028	Cond. No.	4.96e+03

Warnings:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Dealing With the Intercept/Bias

• Two ways of keeping track of the bias term

Dealing With the Intercept/Bias

- Two ways of keeping track of the bias term
- 1. Keep it as a separate parameter:

$$y = w_0 + w_1 x_1 + w_2 x_2 + ... + w_m x_m$$

$$y = w_0 + \sum_{i=1}^m w_i x_i$$

Dealing With the Intercept/Bias

- Two ways of keeping track of the bias term
- 1. Keep it as a separate parameter:

$$y = w_0 + w_1 x_1 + w_2 x_2 + ... + w_m x_m$$

$$y = w_0 + \sum_{i=1}^m w_i x_i$$

2. Append a constant of $x_0 = 1$ so x and w are the same length

$$y = w_0 x_0 + w_1 x_1 + w_2 x_2 + ... + w_m x_m$$

$$y = \sum_{i=0}^{m} w_i x_i$$

```
In [20]: for (name,coef) in zip(['proline','hue'],mlr.coef_):
    print(f'{name:10s} : {coef: 0.3f}')

proline : 0.002
hue : -0.842
```

```
In [20]: for (name, coef) in zip(['proline', 'hue'], mlr.coef_):
              print(f'{name:10s} : {coef: 0.3f}')
          proline
                      : 0.002
                      : -0.842
          hue
In [21]: fig, ax = plt.subplots(1, 2, figsize=(12, 4))
          sns.regplot(x='proline', y='alcohol', data=df_wine, ax=ax[0])
          sns.regplot(x='hue', y='alcohol', data=df_wine, ax=ax[1]);
            15.0
            14.5
                                             12.0
                                             11.5
                                             11.0
```

```
In [20]: for (name, coef) in zip(['proline', 'hue'], mlr.coef_):
              print(f'{name:10s} : {coef: 0.3f}')
          proline
                      : 0.002
          hue
                      : -0.842
In [21]: fig, ax = plt.subplots(1, 2, figsize=(12, 4))
         sns.regplot(x='proline', y='alcohol', data=df_wine, ax=ax[0])
         sns.regplot(x='hue', y='alcohol', data=df_wine, ax=ax[1]);
            15.0
                                            11.5
                                            11.0
```

What would the coefficents look like if the features were on the same scale?

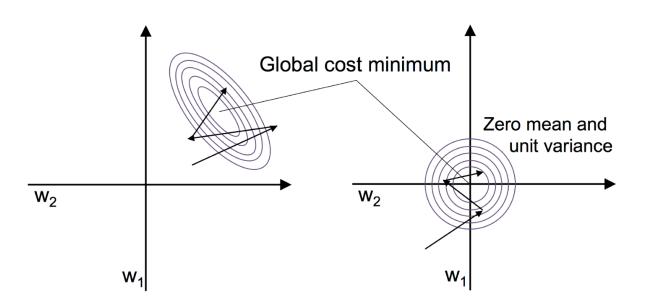
Standardizing/Normalizing Features for Gradient Descent

Standardizing/Normalizing Features for Gradient Descent

$$z = \frac{x - \bar{x}}{s}$$

Standardizing/Normalizing Features for Gradient Descent

$$z = \frac{x - \bar{x}}{s}$$



From PML

• DataFrame.apply():apply a function to each column (axis=0) or each row (axis=1)

• DataFrame.apply():apply a function to each column (axis=0) or each row (axis=1)

```
In [22]: X_zscore = df_wine[['proline','hue']].apply(lambda x: (x-x.mean())/x.std(),axis=0)

mlr_n = LinearRegression()
mlr_n.fit(X_zscore, df_wine.alcohol)
for (name,coef) in zip(X_zscore.columns,mlr_n.coef_):
    print(f'{name:10s} : {coef: 0.3f}')

proline : 0.568
hue : -0.192
```

• DataFrame.apply(): apply a function to each column (axis=0) or each row (axis=1)

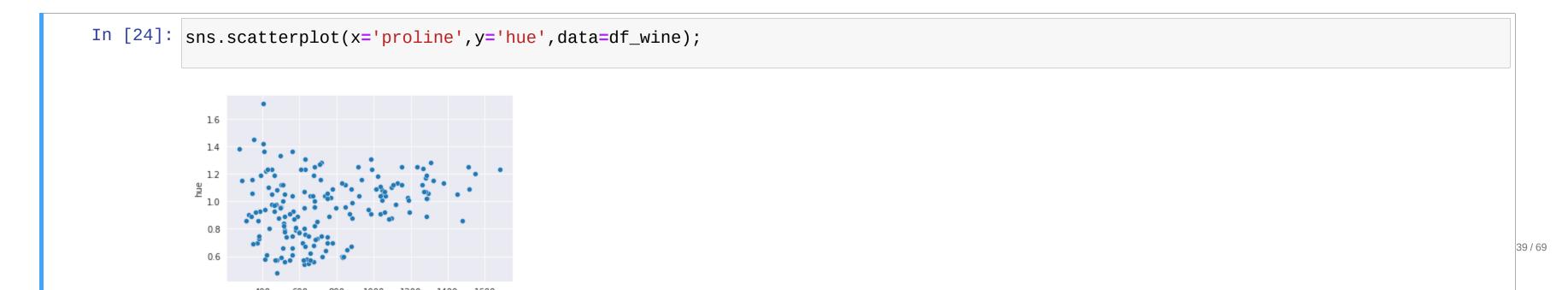
```
In [22]: X_zscore = df_wine[['proline', 'hue']].apply(lambda x: (x-x.mean())/x.std(),axis=0)
         mlr_n = LinearRegression()
         mlr_n.fit(X_zscore, df_wine.alcohol)
         for (name, coef) in zip(X_zscore.columns, mlr_n.coef_):
             print(f'{name:10s} : {coef: 0.3f}')
         proline
                     : 0.568
                     : -0.192
         hue
In [23]: fig, ax = plt.subplots(1, 2, figsize=(12, 4))
         sns.regplot(x=X_zscore.proline,y=df_wine.alcohol,ax=ax[0]);
         sns.regplot(x=X_zscore.hue,y=df_wine.alcohol,ax=ax[1]);
                                           11.5
                                           11.0
                           1.0
```

Colinarity

- MLR assumes features are linearly independent
 - eg: Can't rewrite one column as a weighted sum of the others
 - Ex: in tips dataset: number of entrees ordered will likely be linearly related to table size
- Issue: Model won't know how to estimate w
 - If we add to one w_i and subtract from another, there will be no change in error
- Try to remove obvious colinearity
 - can use correlation and linear regression to detect
 - Important to consider when constructing categorical features (feature engineering)

Colinarity

- MLR assumes features are linearly independent
 - eg: Can't rewrite one column as a weighted sum of the others
 - Ex: in tips dataset: number of entrees ordered will likely be linearly related to table size
- Issue: Model won't know how to estimate w
 - If we add to one w_i and subtract from another, there will be no change in error
- Try to remove obvious colinearity
 - can use correlation and linear regression to detect
 - Important to consider when constructing categorical features (feature engineering)



Aside: Interpretation Vs. Prediction

- Interpretation: Explain how observed features relate to observed target
- Prediction: Given new features, can we generate a prediction

- Often asked to do one or the other, be clear which is most important
- In prediction, may not worry about interpreting the model!

• There is increased attention on interpretability

Questions re Regression with Linear Models?

Classification

- **Regression** -> predict a numeric value
- Classification -> predict a discrete class, category
- Binary classification: two categories
 - pos/neg, cat/dog, win/lose
- Multiclass classification: more than two categories
 - red/green/blue, flower type, integer 0-10
- Multilabel classification: can assign more than one label to an instance
 - paper topics, entities in image

Wine as Binary Classification

Wine as Binary Classification

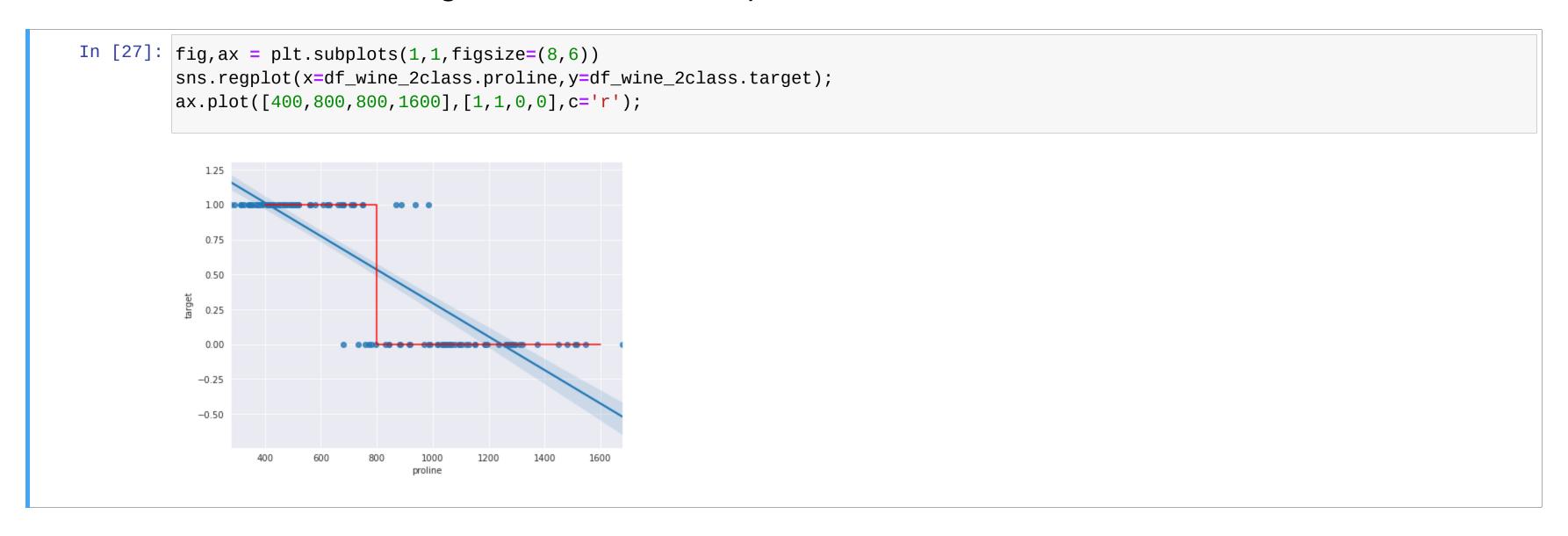
```
In [25]: df_wine['class'].value_counts()

Out[25]: 1 71
0 59
2 48
Name: class, dtype: int64
```

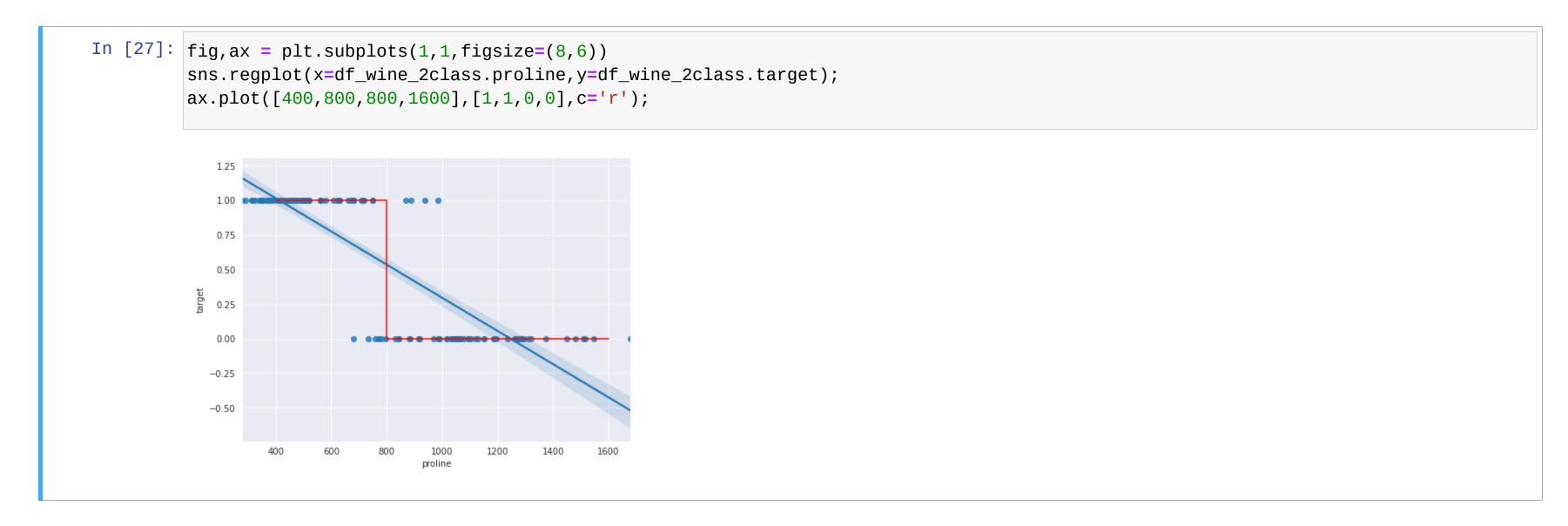
Wine as Binary Classification

• Can't use our linear regression model directly

• Can't use our linear regression model directly



Can't use our linear regression model directly



- Want something with that looks like a threshold
- Would like a prediction between 0 and 1

Logistic Regression

Logistic Regression

$$logistic(x) = \frac{1}{1 + e^{(-x)}}$$

Logistic Regression

$$logistic(x) = \frac{1}{1 + e^{(-x)}}$$

```
In [28]: def logistic(x, w1=1, w0=0):
             return 1 / (1+np.exp(-(w0+w1*x)))
         x = np.linspace(-10, 10, 1000) # generate 1000 numbers evenly spaced between -10 and 10
         fig, ax = plt.subplots(1, 1, figsize=(8, 6))
         ax.plot(x,logistic(x));
         ax.set_xlabel('x');ax.set_ylabel('logistic(x)');
            0.8
            0.2
```

• Our problem becomes: $P(y_i = 1 | x_i) = logistic(w_0 + w_1 x_i) + \varepsilon_i$

• Our problem becomes: $P(y_i = 1 | x_i) = logistic(w_0 + w_1 x_i) + \varepsilon_i$

```
In [29]: from sklearn.linear_model import LogisticRegression

X = df_wine_2class.proline.values.reshape(-1,1)
y = df_wine_2class.target

logr = LogisticRegression(fit_intercept=True).fit(X,y)
print(f'w_0 = {logr.intercept_[0]:0.2f}')
print(f'w_1 = {logr.coef_[0][0]:0.2f}')

w_0 = 11.97
w_1 = -0.01
```

• Our problem becomes: $P(y_i = 1 | x_i) = logistic(w_0 + w_1 x_i) + \varepsilon_i$

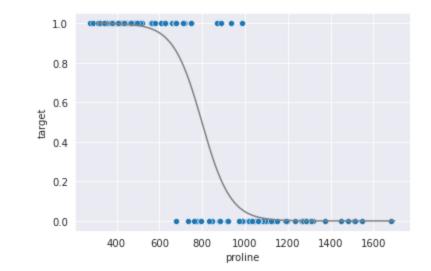
```
In [29]: from sklearn.linear_model import LogisticRegression

X = df_wine_2class.proline.values.reshape(-1,1)
y = df_wine_2class.target

logr = LogisticRegression(fit_intercept=True).fit(X,y)
print(f'w_0 = {logr.intercept_[0]:0.2f}')
print(f'w_1 = {logr.coef_[0][0]:0.2f}')

w_0 = 11.97
w 1 = -0.01
```

```
In [30]: fig,ax = plt.subplots(1,1,figsize=(6,4))
x = np.linspace(300,1700,1000)
logistic_x = logistic(x,logr.coef_[0],logr.intercept_)
ax.plot(x,logistic_x,c='gray');
sns.scatterplot(x=df_wine_2class.proline,y=df_wine_2class.target, ax=ax);
```



Adding the Threshold

Adding the Threshold

- Can treat the output of the logistic function as P(y=1|x)
- Threshold at .5 (50%) to get class prediction

Adding the Threshold

- Can treat the output of the logistic function as P(y = 1 | x)
- Threshold at .5 (50%) to get class prediction

```
In [31]: threshold = x[np.argmin(np.abs(logistic_x - .5))]
         predicted_0 = df_wine_2class[df_wine_2class.proline <= threshold]</pre>
         predicted_1 = df_wine_2class[df_wine_2class.proline > threshold]
         fig, ax = plt.subplots(1, 1, figsize=(6, 4))
         sns.scatterplot(x='proline',y='target', data=predicted_0, color='r',ax=ax);
         sns.scatterplot(x='proline',y='target', data=predicted_1, color='b',ax=ax);
         ax.plot(x,logistic_x,c='gray');
         ax.axvline(threshold, c='k');
            0.8
            0.2
```

Getting Predictions from sklearn

Getting Predictions from sklearn

```
In [32]: yhat = logr.predict(X)
         predicted_0 = df_wine_2class[yhat==0]
         predicted_1 = df_wine_2class[yhat==1]
         fig, ax = plt.subplots(1, 1, figsize=(8, 6))
         sns.scatterplot(x='proline',y='target', data=predicted_0, color='r',ax=ax);
         sns.scatterplot(x='proline',y='target', data=predicted_1, color='b',ax=ax);
         ax.axvline(threshold, c='k');
            0.8
           0.6
            0.2
```

Getting Predictions from sklearn

```
In [32]: yhat = logr.predict(X)
         predicted_0 = df_wine_2class[yhat==0]
         predicted_1 = df_wine_2class[yhat==1]
         fig, ax = plt.subplots(1, 1, figsize=(8, 6))
         sns.scatterplot(x='proline',y='target', data=predicted_0, color='r',ax=ax);
         sns.scatterplot(x='proline',y='target', data=predicted_1, color='b',ax=ax);
         ax.axvline(threshold, c='k');
           0.2
```

Note we have some errors!

• said we could use output of logistic as P(y = 1|x)

• said we could use output of logistic as P(y = 1|x)

• said we could use output of logistic as P(y = 1|x)

```
In [33]: p_y = logr.predict_proba(X)
         p_y[:5] # p(y=0|x), p(y=1|x)
Out[33]: array([[9.81833759e-01, 1.81662409e-02],
                 [9.77356984e-01, 2.26430157e-02],
                 [9.96947414e-01, 3.05258552e-03],
                 [9.99963234e-01, 3.67664871e-05],
                 [2.77482032e-01, 7.22517968e-01]])
In [34]: plt.scatter(df_wine_2class.proline,p_y[:,1]);
          0.8
           0.6
          0.4
          0.2
```

Interpreting Logistic Regression Coefficients

After some math

$$\log\left(\frac{y_i}{1-y_i}\right) = w_0 + w_1 x_{i1}$$

- this is the **log odds ratio** of p(y=1)/p(y=0)
- odds range from 0 to positive infinity
- odds(5) -> 5/1 -> 5 out of 6 times -> .83
- odds(.2) -> 1/5 -> 1 out of 6 times -> .16

See <u>here</u> for a good explanation

Logistic Regression with Multiple Features

Logistic Regression with Multiple Features

```
In [35]: X = df_wine_2class[['proline', 'hue']]
X_zscore = X.apply(lambda x: (x-x.mean())/x.std())

logrm = LogisticRegression().fit(X_zscore, y)
for (name, coef) in zip(X.columns, logrm.coef_[0]):
    print(f'{name:10s} : {coef: 0.3f}')

proline : -3.464
hue : 0.488
```

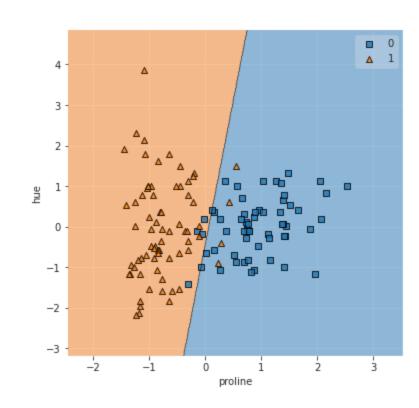
Logistic Regression with Multiple Features

```
In [35]: X = df_wine_2class[['proline', 'hue']]
X_zscore = X.apply(lambda x: (x-x.mean())/x.std())
logrm = LogisticRegression().fit(X_zscore,y)
for (name,coef) in zip(X.columns,logrm.coef_[0]):
    print(f'{name:10s} : {coef: 0.3f}')

proline : -3.464
hue : 0.488

In [36]: # need to have run: conda install -n eods-f20 -c conda-forge mlxtend
from mlxtend.plotting import plot_decision_regions

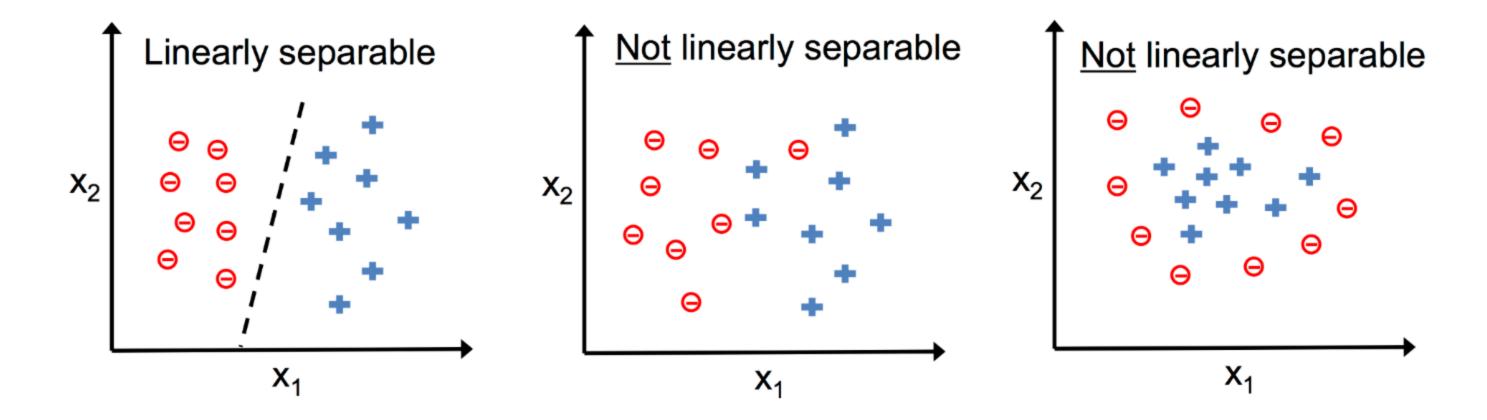
fig,ax = plt.subplots(1,1,figsize=(6,6))
    plot_decision_regions(X_zscore.values, y.values, clf=logrm, ax=ax);
    ax.set_xlabel(X.columns[0]); ax.set_ylabel(X.columns[1]);
```



Linearly Seperable Data

Linearly Seperable Data

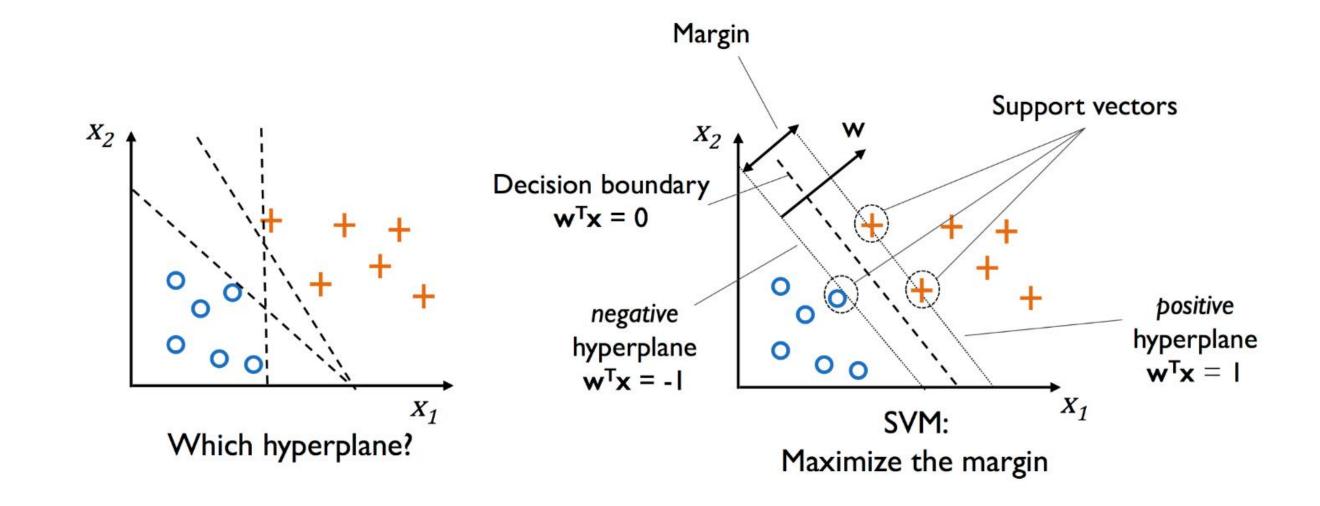
• Logistic Regression depends on data being linearly seperable



From PML

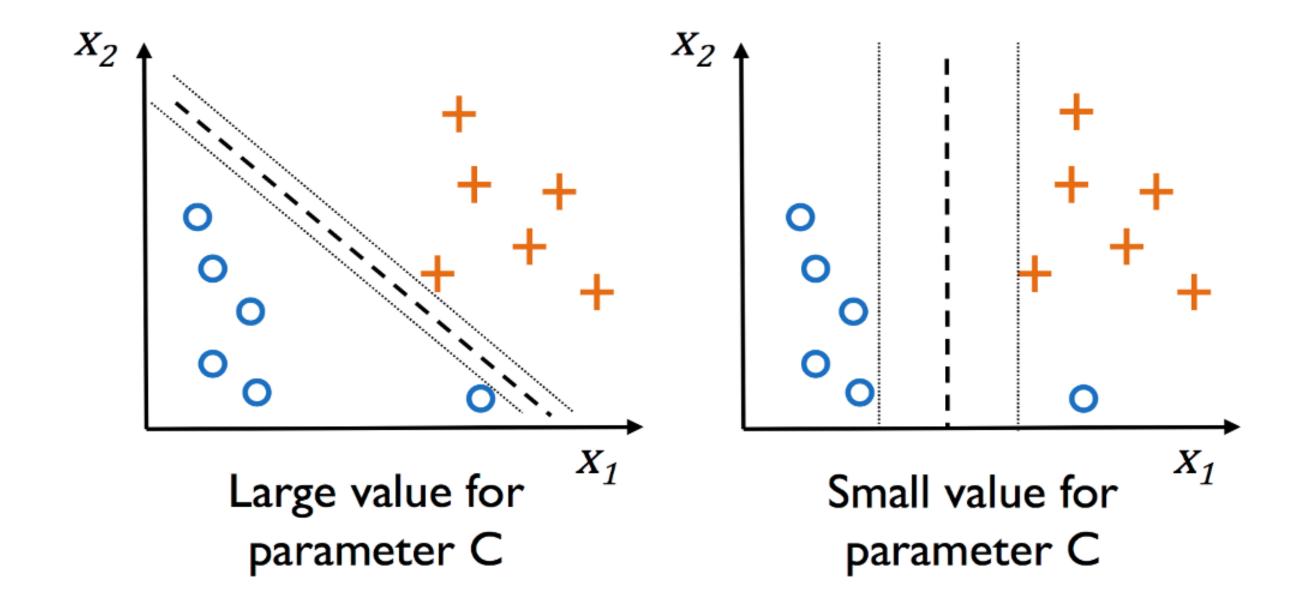
Which boundary should we use? Support Vector Machines (SVMs)

- For a linearly seperable dataset, where should we place the decision boundary?
- Support Vector Machine (SVM) tries to "maximize the margin" between classes



SVM Hyperparameter C

• Hyperparameter: Something we set



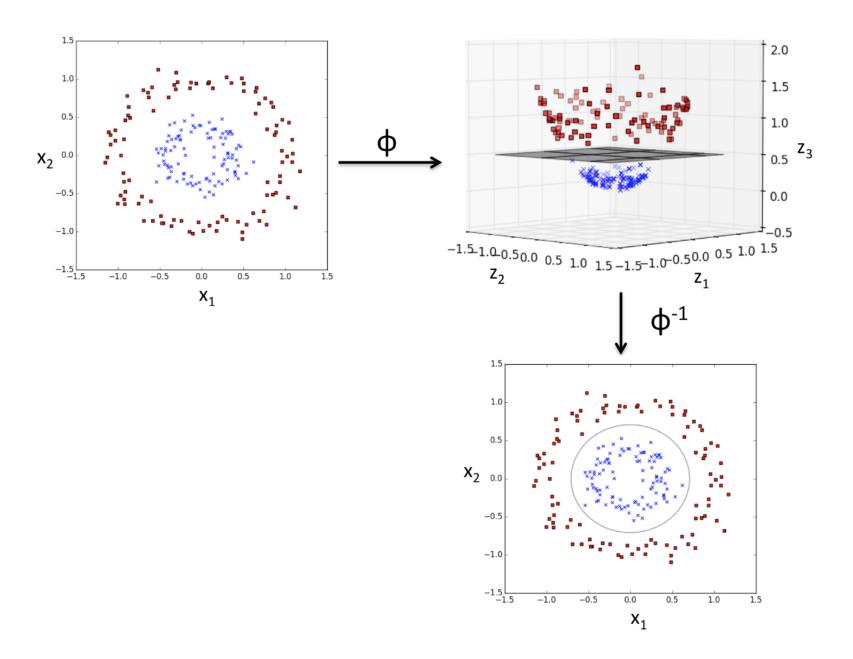
SVM with sklearn

SVM with sklearn

```
In [37]: from sklearn.svm import SVC
         svm_linear = SVC(kernel='linear')
         svm_linear.fit(X_zscore,y);
         fig,ax = plt.subplots(1,1,figsize=(6,6))
         plot_decision_regions(X_zscore.values, y.values, clf=svm_linear);
         plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```

Non-Linear Boundaries with SVMs Kernel Trick

• Kernel Trick: Map data to a higher dimensional space and find linear boundary there



SVM Kernel Trick with RBF Kernel

SVM Kernel Trick with RBF Kernel

• RBF (Radial-Basis Function) kernel

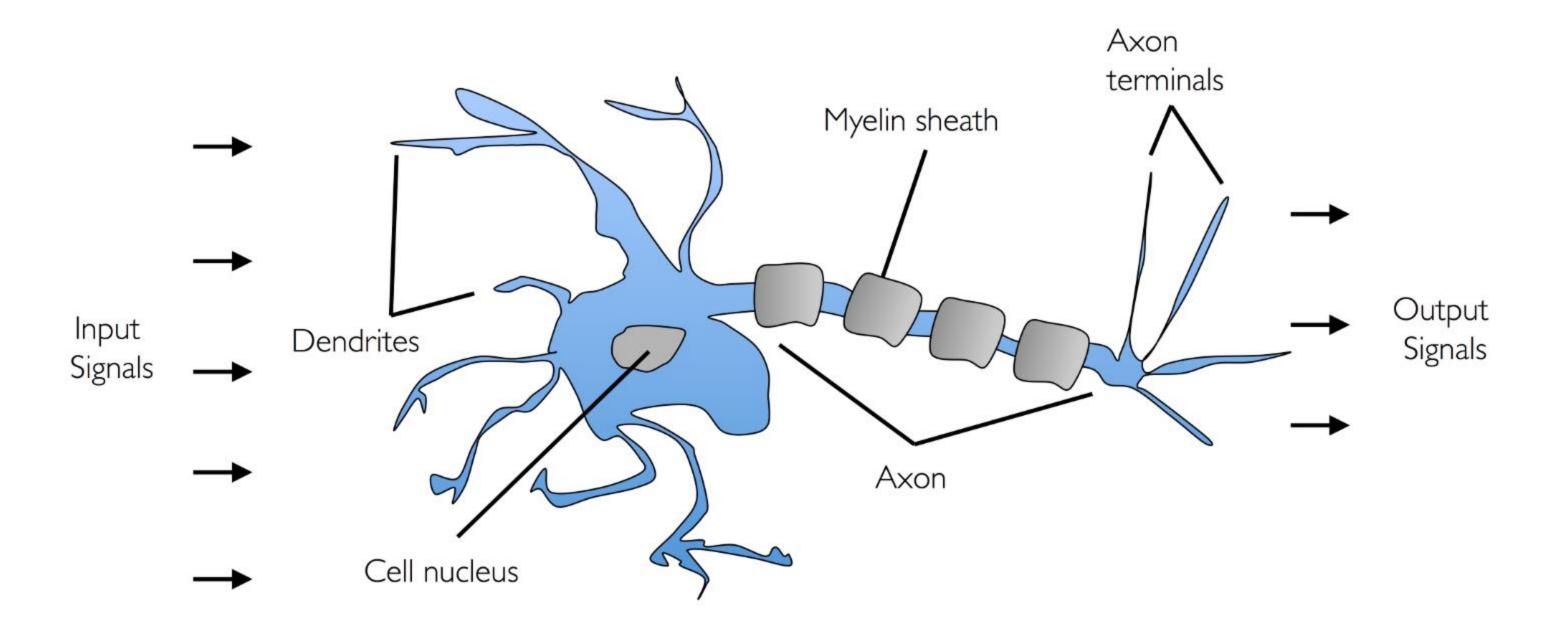
SVM Kernel Trick with RBF Kernel

• RBF (Radial-Basis Function) kernel

```
In [38]: svm_rbf = SVC(kernel='rbf')
         svm_rbf.fit(X_zscore,y);
         fig,ax = plt.subplots(1,1,figsize=(6,6))
         plot_decision_regions(X_zscore.values, y.values, clf=svm_rbf);
         plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```

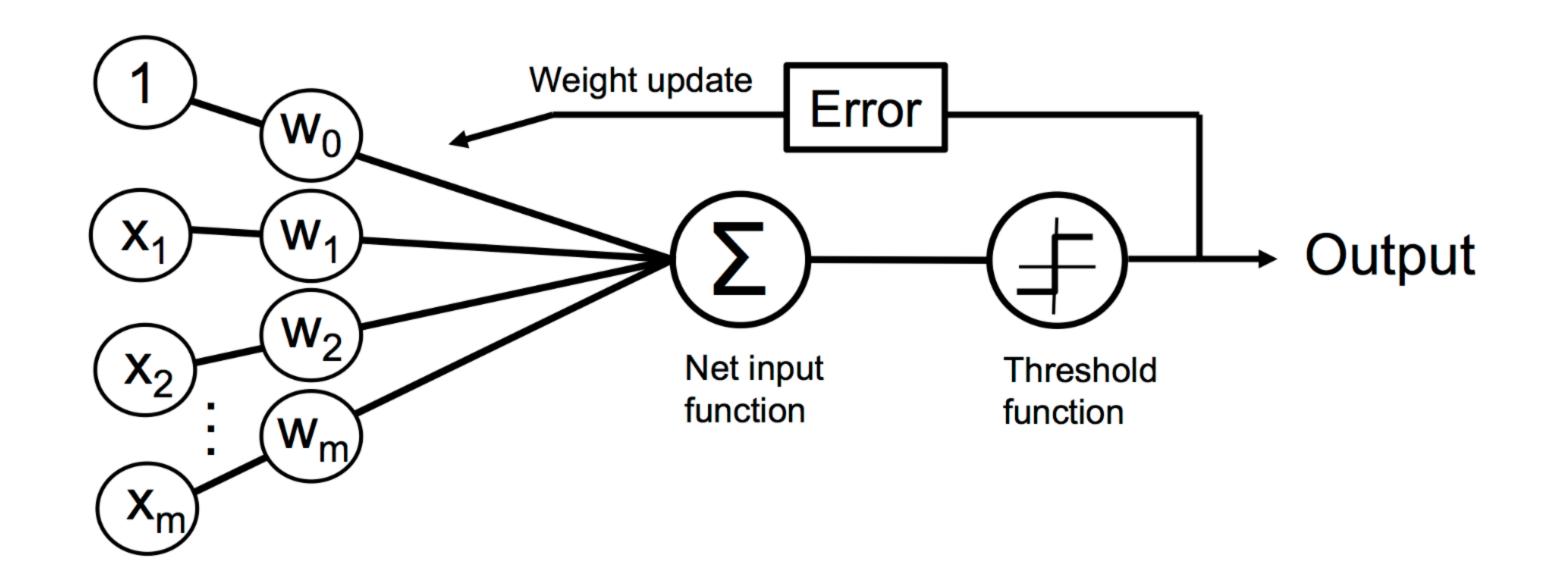
If we have time...

From Perceptron to Artificial Neural Network



From PML

Perceptron: Early Neuron Model



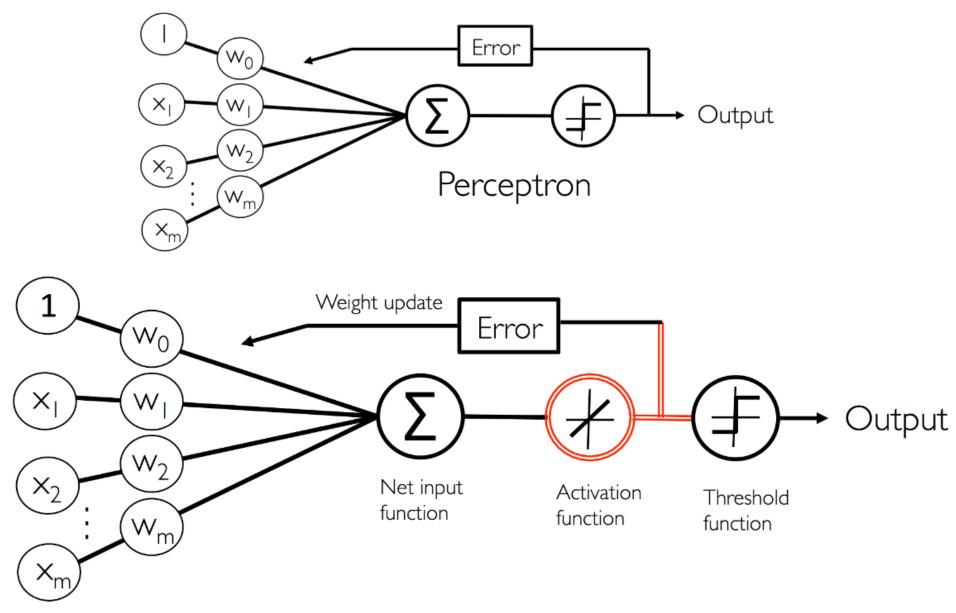
From PML

Perceptron in sklearn

Perceptron in sklearn

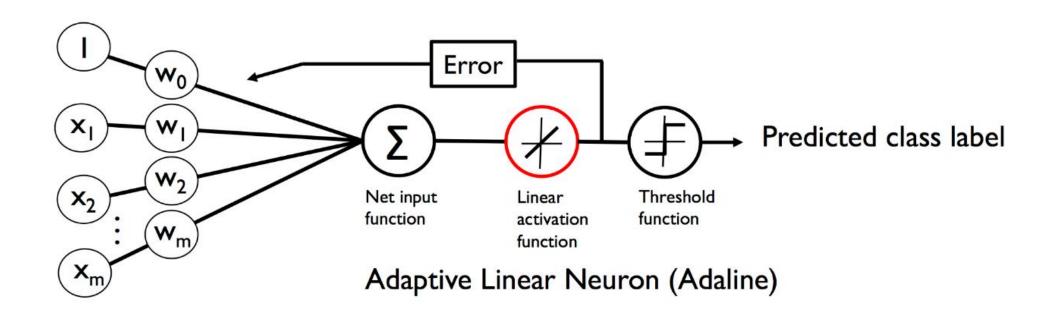
```
In [39]: from sklearn.linear_model import Perceptron
         perceptron = SVC(kernel='linear')
         perceptron.fit(X_zscore,y);
         fig, ax = plt.subplots(1, 1, figsize=(6, 6))
         plot_decision_regions(X_zscore.values, y.values, clf=perceptron);
         plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```

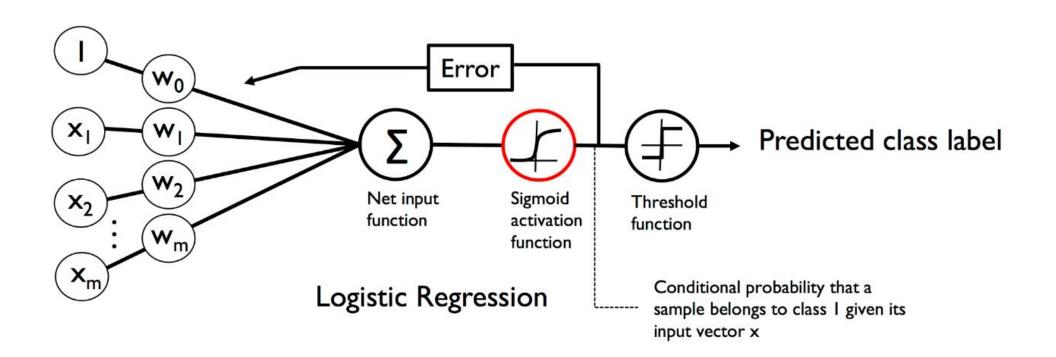
Perceptron to Adaline



Adaptive Linear Neuron (Adaline)

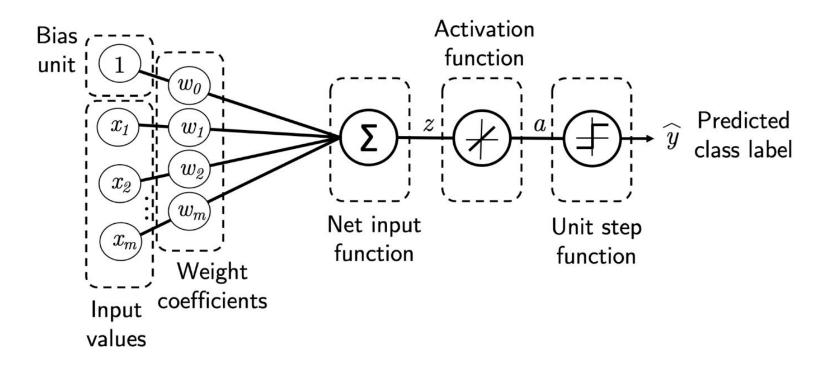
Adaline to Linear Regression



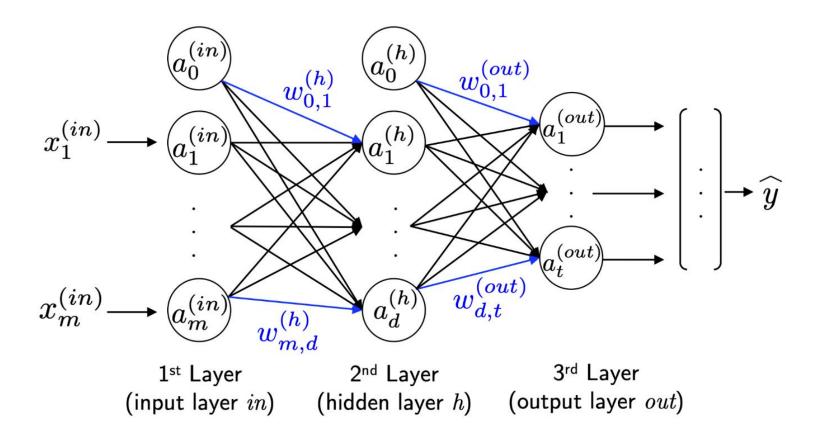


From PML 63/69

Components of Single Layer Neural Net

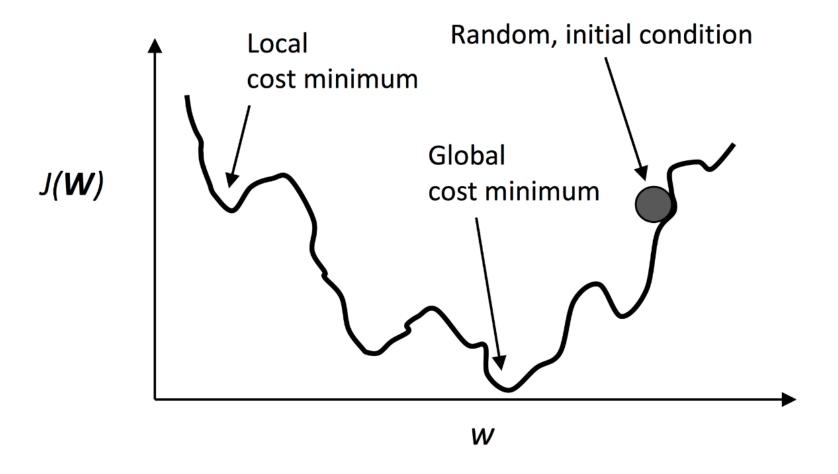


Multi-Layer Neural Network



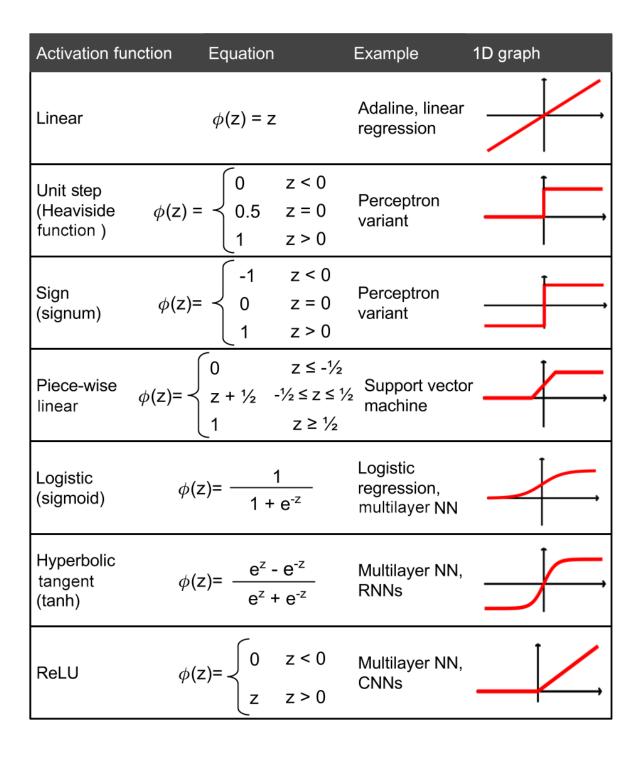
From PML

Complex Optimization Space



From PML

Activation Functions



Multi-Layer Perceptron with sklearn

Multi-Layer Perceptron with sklearn

```
In [40]: from sklearn.neural_network import MLPClassifier, MLPRegressor
         mlp = MLPClassifier(hidden_layer_sizes=(100,),
                             max_iter=1000)
         mlp.fit(X_zscore,y);
         fig,ax = plt.subplots(1,1,figsize=(6,6))
         plot_decision_regions(X_zscore.values, y.values, clf=mlp);
         plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```

Questions re Classification with Linear Models?