Elements Of Data Science - F2022

Week 9: Dimensionality Reduction, Feature Selection and Feature Extraction

11/2/2022

TODOs

- Readings:
 - PML Chapter 6.1, Streamlining workflows with Pipelines
 - PML Chapter 8: Applying Machine Learning to Sentiment Analysis
- HW 2, Due Fri Nov 4th, 11:59pm ET
- Quiz 9, Due Tues Nov 8th, 11:59pm ET
- HW3 Out Friday, due Nov 18th

Quiz 7 Notes

• Be careful which dataset you're training/evaluating on: X_train vs X_test

Today

- Joining Datasets
- Dimensionality Reduction
 - Feature Selection
 - Linear Model with LASSO
 - Tree Based Models Feature Importance
 - Univariate Tests
 - Recursive Feature Selection
 - Aside: Adjusted *R*²
 - Feature Extraction
 - o PCA
- Example: Image Recognition Using PCA

Questions?

Environment Setup

Environment Setup

```
In [1]: import numpy
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

from mlxtend.plotting import plot_decision_regions

sns.set_style('darkgrid')
%matplotlib inline
```

Joing Datasets

• often have two sets of data we need to join together

Joing Datasets

• often have two sets of data we need to join together

Joing Datasets

• often have two sets of data we need to join together

```
In [3]: df_flower_name_orig = pd.DataFrame([[1001, 'iris'], [1002, 'rose']],
                                              columns=['flower_id', 'name'])
        df_flower_price_orig = pd.DataFrame([[1002,3.99],[1003,2.25]],
                                               columns=['flower_id','price'])
In [4]: display(df_flower_name_orig)
        display(df_flower_price_orig)
            flower_id name
                    iris
         0 1001
         1 1002
                    rose
            flower_id price
         0 1002
                    3.99
                   2.25
         1 1003
```

Joing Datasets On Index

- easiest way to join Pandas DataFrames is on row index label
- may need to set the index from a column using .set_index()

Joing Datasets On Index

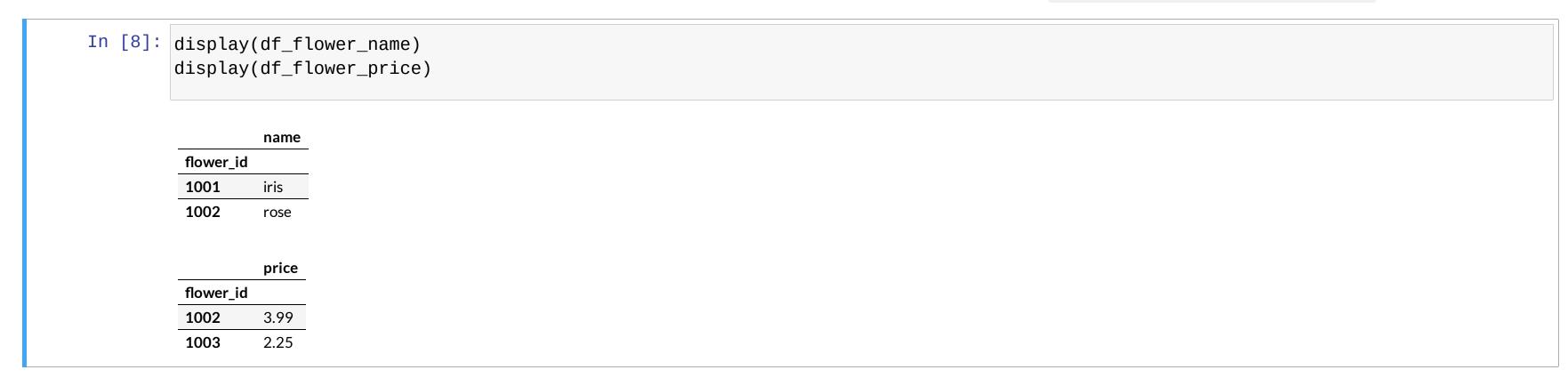
- easiest way to join Pandas DataFrames is on row index label
- may need to set the index from a column using .set_index()

```
In [5]: df_flower_name_orig
Out[5]:
            flower_id name
                    iris
          0 1001
          1 1002
                    rose
In [6]: df_flower_name = df_flower_name_orig.set_index('flower_id') # note: inplace=False, drop=True by default
        df_flower_name
Out[6]:
                 name
          flower_id
          1001
                 iris
          1002
                 rose
```

Joing Datasets On Index

- easiest way to join Pandas DataFrames is on row index label
- may need to set the index from a column using .set_index()

```
In [5]: df_flower_name_orig
Out[5]:
            flower_id name
                    iris
          0 1001
          1 1002
                    rose
In [6]: df_flower_name = df_flower_name_orig.set_index('flower_id') # note: inplace=False, drop=True by default
         df_flower_name
Out[6]:
                  name
          flower id
          1001
                  iris
          1002
                  rose
In [7]: df_flower_price = df_flower_price_orig.set_index('flower_id')
         df_flower_price
Out[7]:
                  price
          flower id
                  3.99
          1002
                  2.25
          1003
```

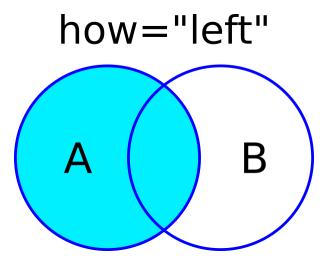


```
In [8]: display(df_flower_name)
         display(df_flower_price)
                   name
          flower_id
                   iris
          1001
          1002
                   rose
                   price
          flower_id
                   3.99
          1002
                  2.25
          1003
In [9]: df_flower_name.join(df_flower_price)
Out[9]:
                   name price
          flower_id
                        NaN
          1001
                   iris
                        3.99
          1002
                   rose
```

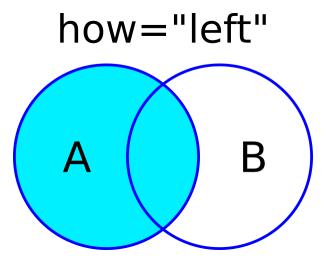


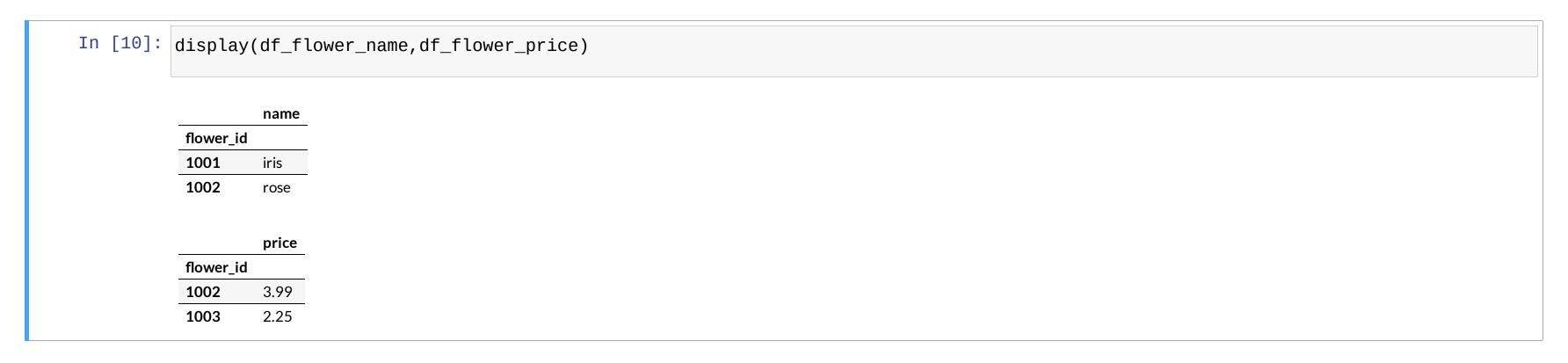
• by default, this is a 'Left Join'

Join Types: Left Join

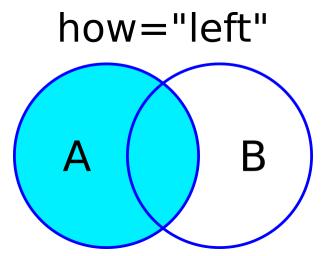


Join Types: Left Join





Join Types: Left Join



In [10]: display(df_flower_name, df_flower_price)

	name
flower_id	
1001	iris
1002	rose

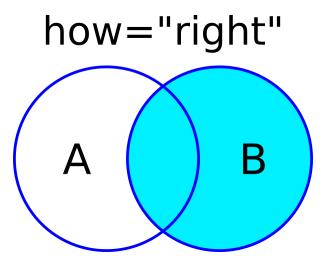
flower_id 3.99
1003 2.25

In [11]: df_flower_name.join(df_flower_price,how="left") # default for df.join() is left join

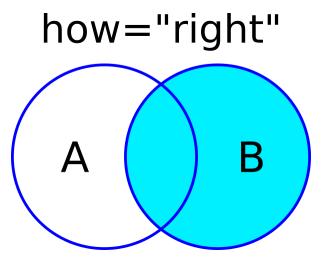
Out[11]:

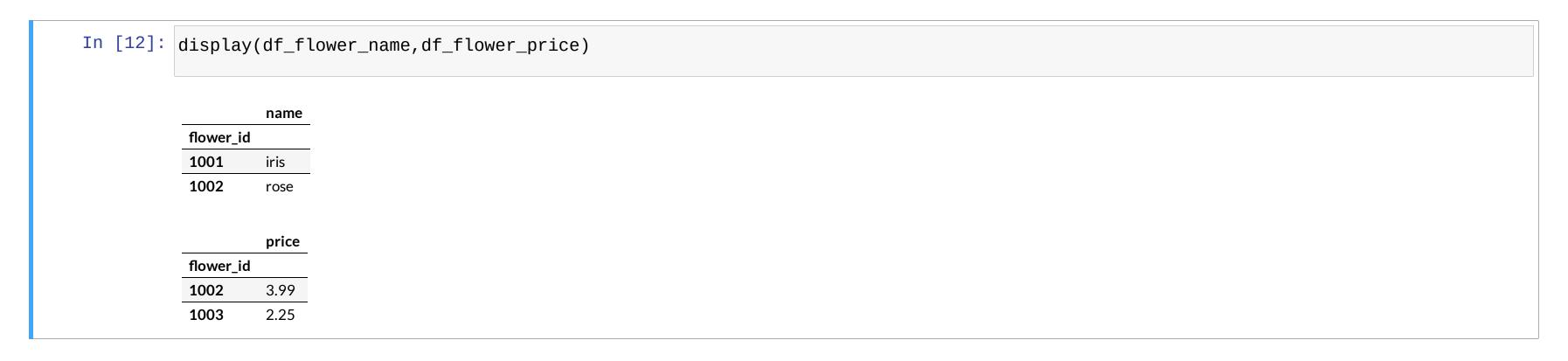
	name	price
flower_id		
1001	iris	NaN
1002	rose	3.99

Join Types: Right Join

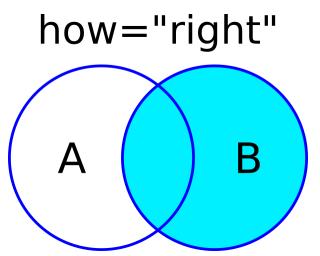


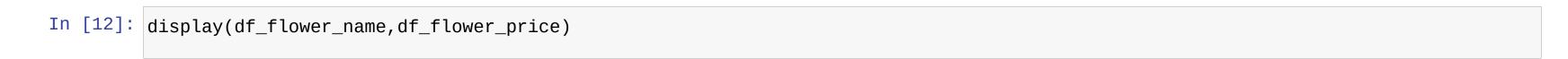
Join Types: Right Join





Join Types: Right Join





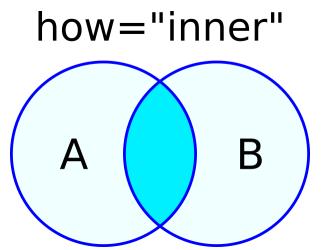
	name
flower_id	
1001	iris
1002	rose

```
In [13]: df_flower_name.join(df_flower_price,how='right')
```

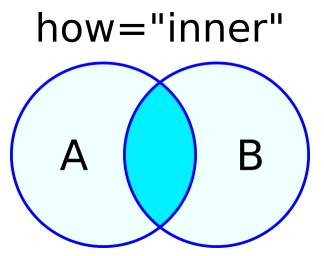
Out[13]:

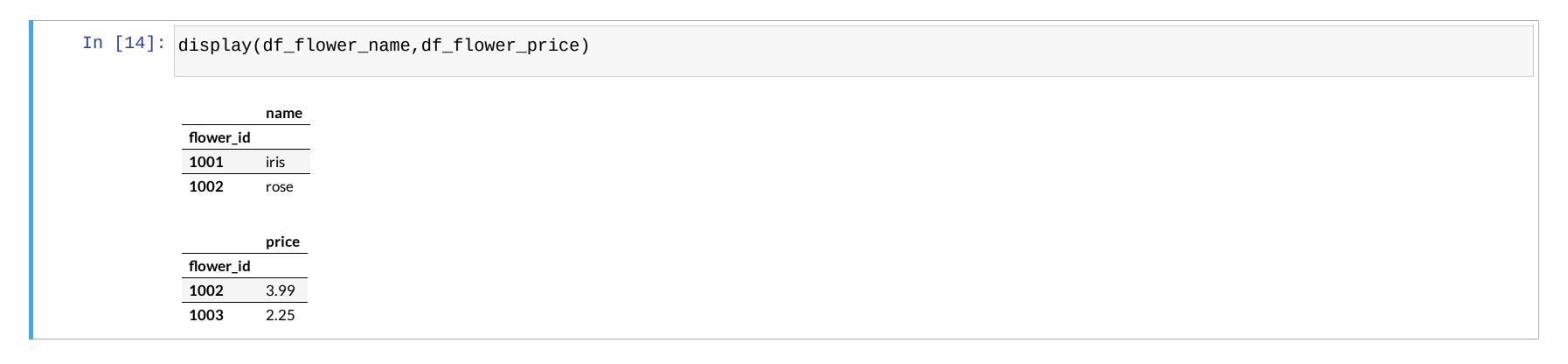
	name	price
flower_id		
1002	rose	3.99
1003	NaN	2.25

Join Types: Inner Join

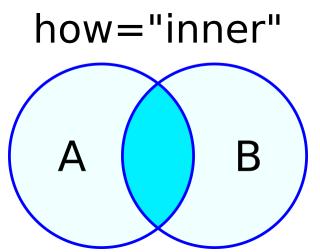


Join Types: Inner Join





Join Types: Inner Join

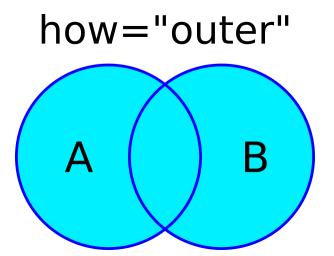




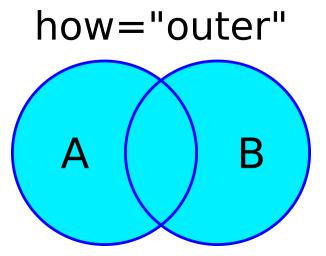
	name
flower_id	
1001	iris
1002	rose

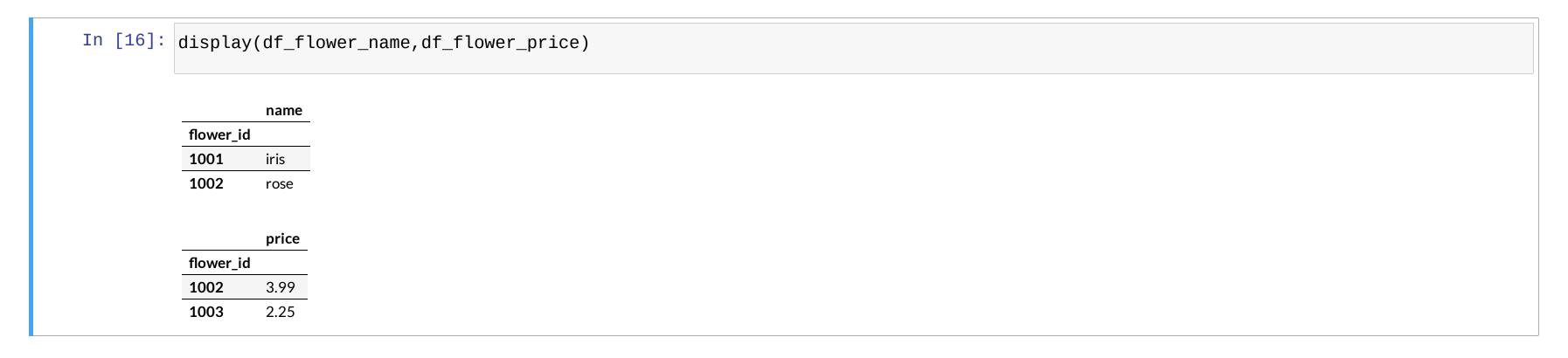
flower_id 3.99
1003 2.25

Join Types: Outer Join

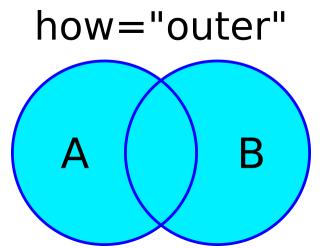


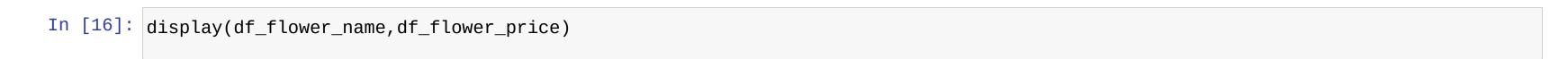
Join Types: Outer Join





Join Types: Outer Join





	name
flower_id	
1001	iris
1002	rose

flower_id 3.99 1003 2.25

```
In [17]: df_flower_name.join(df_flower_price, how='outer')
```

Out[17]:

	name	price
flower_id		
1001	iris	NaN
1002	rose	3.99
1003	NaN	2.25

Setting the Index When Reading in Data

• instead of using .set_index(), can specify index_col=on .read functions

Setting the Index When Reading in Data

• instead of using .set_index(), can specify index_col=on .read functions

```
In [18]: # this csv has column for purchase_id
pd.read_csv('../data/flowershop_data_with_dups.csv'
).head(2)

Out[18]:

purchase_id lastname purchase_date stars price favorite_flower

0 1000 PERKINS 2017-04-08 5 19.599886 iris

1 1001 ROBINSON 2017-01-01 5 37.983904 NaN
```

Setting the Index When Reading in Data

• instead of using .set_index(), can specify index_col=on .read functions

```
In [18]: # this csv has column for purchase_id
          pd.read_csv('../data/flowershop_data_with_dups.csv'
                       ).head(2)
Out[18]:
              purchase id
                          lastname purchase_date stars
                                                       price favorite flower
                        PERKINS
                                  2017-04-08
                                                   19.599886 iris
           0 1000
           1 1001
                        ROBINSON 2017-01-01
                                                   37.983904 NaN
In [19]: # can set the index when reading in the csv
          pd.read_csv('../data/flowershop_data_with_dups.csv',
                       index_col='purchase_id'
                                                                      # set the index column when reading/loading data
                      ).head(2)
Out[19]:
                       lastname purchase date stars
                                                     price favorite flower
           purchase id
           1000
                      PERKINS
                               2017-04-08
                                                 19.599886 iris
                                                 37.983904 NaN
           1001
                      ROBINSON 2017-01-01
```

```
In [20]: # imagine that 'name' is a categorical variable df_flower_name[['name']]

Out[20]:

name
flower_id
1001 iris
1002 rose
```

```
In [20]: # imagine that 'name' is a categorical variable
          df_flower_name[['name']]
Out[20]:
                   name
           flower_id
           1001
           1002
                   rose
In [21]: # converting categorical to one-hot using get_dummies
          pd.get_dummies(df_flower_name['name'], prefix='flower_name')
Out[21]:
                  flower_name_iris flower_name_rose
          flower_id
           1001
          1002
                   0
```

```
In [20]: # imagine that 'name' is a categorical variable
          df_flower_name[['name']]
Out[20]:
                   name
           flower id
           1001
           1002
                   rose
In [21]: # converting categorical to one-hot using get_dummies
          pd.get_dummies(df_flower_name['name'], prefix='flower_name')
Out[21]:
                  flower_name_iris flower_name_rose
           flower_id
           1001
                   0
           1002
In [22]: # can join back using the default index
          df_flower_name[['name']].join(pd.get_dummies(df_flower_name['name'],prefix='flower_name'))
Out[22]:
                  name flower_name_iris flower_name_rose
           flower_id
           1001
                   iris
                       1
           1002
                   rose
```

Join on Columns Instead of Index using pd.merge()

• to do more complicated joins, use pd.merge()

Join on Columns Instead of Index using pd.merge()

• to do more complicated joins, use pd.merge()

Join on Columns Instead of Index using pd.merge()

• to do more complicated joins, use pd.merge()

```
In [23]: # using the dataframes before setting index using .set_index()
         pd.merge(df_flower_name_orig,
                   df_flower_price_orig,
                   left_on='flower_id',
                   right_on='flower_id') # what is the default join for merge?
Out[23]:
             flower_id name price
                    rose 3.99
          0 1002
In [24]: # if both id columns have the same name, can just use "on="
         pd.merge(df_flower_name_orig,
                   df_flower_price_orig,
                   on='flower_id',
                   how='outer')
Out[24]:
             flower_id name price
          0 1001
                    iris
                         NaN
          1 1002
                    rose
                         3.99
          2 1003
                    NaN 2.25
```

Joining Datasets Review

- Use .join() when you can, joining on Pandas DataFrame row index labels
- May need to set the dataframe row index labels
 - index_col= when creating the DataFrame or
 - set_index() after DataFrame creation
- Know the different general join types: Left, Right, Inner, Outer
- Use pd.merge() when you need something more complex than joining on row index

Questions about joining datasets?

Dimensionality Reduction

Recall: Methods for Avoiding Overfitting

- Collect additional examples
- Use a simple model
- Regularization
- Reduce the dimensions of our data: Dimensionality Reduction

Dimensionality Reduction

- Reasons to reduce the number of features:
 - improve model performance (reduce complexity to reduce chance of overfitting)
 - improve speed performance (reduce number of calculations)
 - interpretation (which features are most important?)

Feature Selection

choose a subset of original features

Feature Extraction

combine/transform features to generate a new feature space

Load Binary Wine Classification

Load Binary Wine Classification

```
In [25]: from sklearn.datasets import load_wine
                                   from sklearn.model_selection import train_test_split
                                   wine = load_wine()
                                   X_wine = pd.DataFrame(wine.data,columns=wine.feature_names)
                                   y_wine = wine.target
                                   # reduce to binary classification
                                  X_wine = X_wine.iloc[y_wine < 2]</pre>
                                   y_wine = y_wine[y_wine < 2]</pre>
                                  X_{train}, X_{test}, y_{train}, y_{test} = train_{test}, y_{train}, x_{test}, y_{train}, y_{test} = train_{test}, y_{train}, x_{test}, y_{train}, y_{test} = train_{test}, y_{train}, y_{test}, y_{train}, y_{test} = train_{test}, y_{train}, y_{test}, y_{train}, y_{test} = train_{test}, y_{train}, y_{test}, y_{test}
                                   wine feature names = X wine.columns.values
                                   wine_feature_names
Out[25]: array(['alcohol', 'malic_acid', 'ash', 'alcalinity_of_ash', 'magnesium',
                                                                 'total_phenols', 'flavanoids', 'nonflavanoid_phenols',
                                                                'proanthocyanins', 'color_intensity', 'hue',
                                                                'od280/od315_of_diluted_wines', 'proline'], dtype=object)
```

Load Binary Wine Classification

86 12.16

121 11.56

30 13.73

1.61

2.05

1.50

2.31 22.8

3.23 28.5

2.70 22.5

90.0

119.0

101.0

1.78

3.18

3.00

```
In [25]: from sklearn.datasets import load_wine
                              from sklearn.model_selection import train_test_split
                              wine = load_wine()
                              X_wine = pd.DataFrame(wine.data,columns=wine.feature_names)
                              y_wine = wine.target
                              # reduce to binary classification
                             X_wine = X_wine.iloc[y_wine < 2]</pre>
                              y_wine = y_wine[y_wine < 2]
                             X_train, X_test, y_train, y_test = train_test_split(X_wine, y_wine, stratify=y_wine, random_state=0)
                              wine_feature_names = X_wine.columns.values
                              wine_feature_names
Out[25]: array(['alcohol', 'malic_acid', 'ash', 'alcalinity_of_ash', 'magnesium',
                                                       'total_phenols', 'flavanoids', 'nonflavanoid_phenols',
                                                       'proanthocyanins', 'color_intensity', 'hue',
                                                       'od280/od315_of_diluted_wines', 'proline'], dtype=object)
In [26]: X_train.head(3)
 Out[26]:
                                               alcohol malic_acid ash alcalinity_of_ash magnesium total_phenols flavanoids nonflavanoid_phenols proanthocyanins color_intensity hue od280/od315_of_diluted_wines proanthocyaning hue od280/od316_of_diluted_wines proanthocyang hue od280/od316_of_diluted_wines proanthocyaning hue od280/od3
```

1.69

5.08

3.25

0.43

0.47

0.29

1.56

1.87

2.38

2.45

6.00

5.70

1.33 2.26

0.93 3.69

1.19 2.71

49!

46!

128

Need to Standardize Features

Need to Standardize Features

```
In [27]: X_train.agg(['mean', 'std']).transpose().round(1)
Out[27]:
                                               std
                                        mean
                                             0.9
                                       13.0
            alcohol
                                       2.0
                                             0.9
            malic_acid
                                             0.3
                                       2.4
            ash
            alcalinity_of_ash
                                       19.1
                                             3.7
                                             15.0
                                       99.1
            magnesium
            total_phenols
                                       2.5
                                             0.5
            flavanoids
                                       2.5
                                             8.0
            nonflavanoid_phenols
                                       0.3
                                             0.1
            proanthocyanins
                                       1.8
                                             0.6
            color_intensity
                                       4.2
                                             1.7
            hue
                                       1.1
                                             0.2
            od280/od315_of_diluted_wines 2.9
                                             0.5
                                       803.1 363.2
            proline
```

Standardize Features

Standardize Features

```
In [28]: from sklearn.preprocessing import StandardScaler

ss = StandardScaler()
X_train_zscore = ss.fit_transform(X_train)
X_train_zscore = pd.DataFrame(X_train_zscore, columns=wine_feature_names)

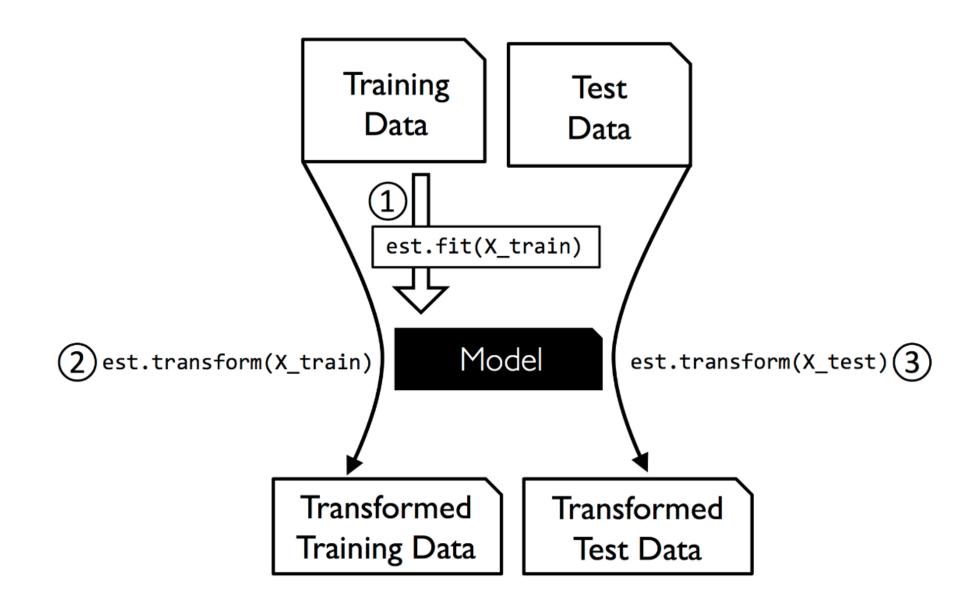
X_test_zscore = ss.transform(X_test)
```

Standardize Features

```
In [28]: from sklearn.preprocessing import StandardScaler
          ss = StandardScaler()
          X_train_zscore = ss.fit_transform(X_train)
          X_train_zscore = pd.DataFrame(X_train_zscore, columns=wine_feature_names)
          X_test_zscore = ss.transform(X_test)
In [29]: X_train_zscore.agg(['mean', 'std']).T.round(1)
Out[29]:
                                    mean std
           alcohol
                                    -0.0
                                         1.0
           malic acid
                                    -0.0
                                         1.0
                                         1.0
           ash
                                    0.0
           alcalinity_of_ash
                                         1.0
                                    -0.0
                                        1.0
           magnesium
                                    0.0
           total_phenols
                                         1.0
                                    0.0
                                   0.0
                                         1.0
           flavanoids
           nonflavanoid_phenols
                                    -0.0
                                         1.0
                                         1.0
           proanthocyanins
                                    0.0
           color_intensity
                                    0.0
                                         1.0
                                    -0.0
                                        1.0
           hue
           od280/od315_of_diluted_wines -0.0
                                         1.0
                                    -0.0 1.0
           proline
```

Recall: Predicting vs Transforming with Train/Test Split

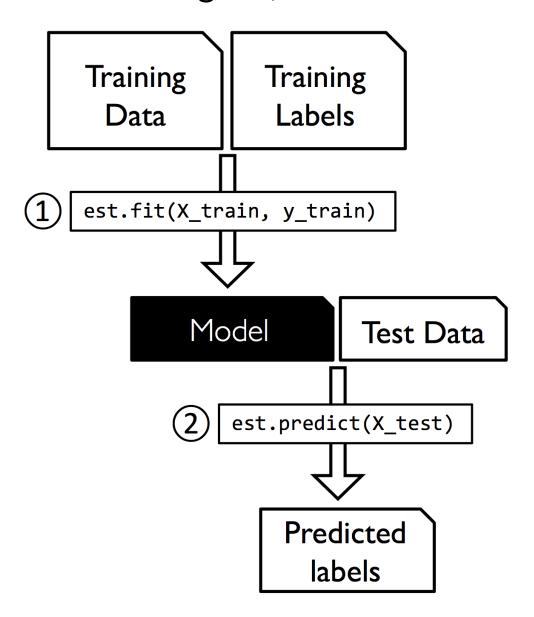
- When transforming data, fit on the training set, transform both train and test



From PML

Recall: Predicting vs Transforming with Train/Test Split

- When performing prediction, train on the training set, evaluate on the test set



From PML

Feature Selection

- Select a subset of features
- Based on how much they contribute to predicting the target 'y'

Feature Selection

- Select a subset of features
- Based on how much they contribute to predicting the target 'y'
- From a Model
 - Linear Model with LASSO Regularization
 - Tree Based Models Feature Importance
- Univariate Tests
- Recursive Feature Selection

Feature Selection: LASSO (L1)

• LASSO or ℓ_1 or 11 regularization drives the coefficient of uninformative features to 0

Feature Selection: LASSO (L1)

• LASSO or ℓ_1 or 11 regularization drives the coefficient of uninformative features to 0

Feature Selection: LASSO (L1)

• LASSO or ℓ_1 or 11 regularization drives the coefficient of uninformative features to 0

```
In [30]: from sklearn.linear_model import LogisticRegression
         # First, without regularization
         # C is the inverse regularization strength: higher means less regularization
         logr = LogisticRegression(penalty="none", solver="lbfgs", random_state=0)
         logr.fit(X_train_zscore, y_train)
         logr.coef_[0].round(2)
Out[30]: array([ -8.14, -4.41, -8.11, 11.54, -2.72, 2.24, -3.52, 1.05,
                  0.91, -1.55, 0.2, -3.87, -14.43
In [31]: pd.Series(logr.coef [0],index=wine feature names).sort values(ascending=False).round(2)
Out[31]: alcalinity_of_ash
                                        11.54
         total phenols
                                          2.24
         nonflavanoid_phenols
                                         1.05
         proanthocyanins
                                         0.91
                                         0.20
         hue
         color intensity
                                         -1.55
                                         -2.72
         magnesium
                                         -3.52
         flavanoids
         od280/od315 of diluted wines
                                         -3.87
         malic_acid
                                         -4.41
                                         -8.11
         ash
         alcohol
                                         -8.14
         proline
                                        -14.43
         dtype: float64
```

Feature Selection: LASSO (L1) Cont.

Feature Selection: LASSO (L1) Cont.

```
In [32]: # Now with LASSO
         logr_l1 = LogisticRegression(C=0.1, penalty="l1", solver="liblinear", random_state=0)
         logr_l1.fit(X_train_zscore, y_train)
         pd.Series(logr_l1.coef_[0],index=wine_feature_names).sort_values(ascending=False).round(5)
Out[32]: malic acid
                                         0.00000
                                         0.00000
         ash
         alcalinity_of_ash
                                         0.00000
         magnesium
                                         0.00000
         total_phenols
                                         0.00000
         flavanoids
                                         0.00000
         nonflavanoid_phenols
                                         0.00000
         proanthocyanins
                                         0.00000
         color_intensity
                                         0.00000
                                         0.00000
         hue
         od280/od315 of diluted wines
                                         0.00000
         alcohol
                                        -0.66710
         proline
                                        -1.37284
         dtype: float64
```

Feature Selection: LASSO (L1) Cont.

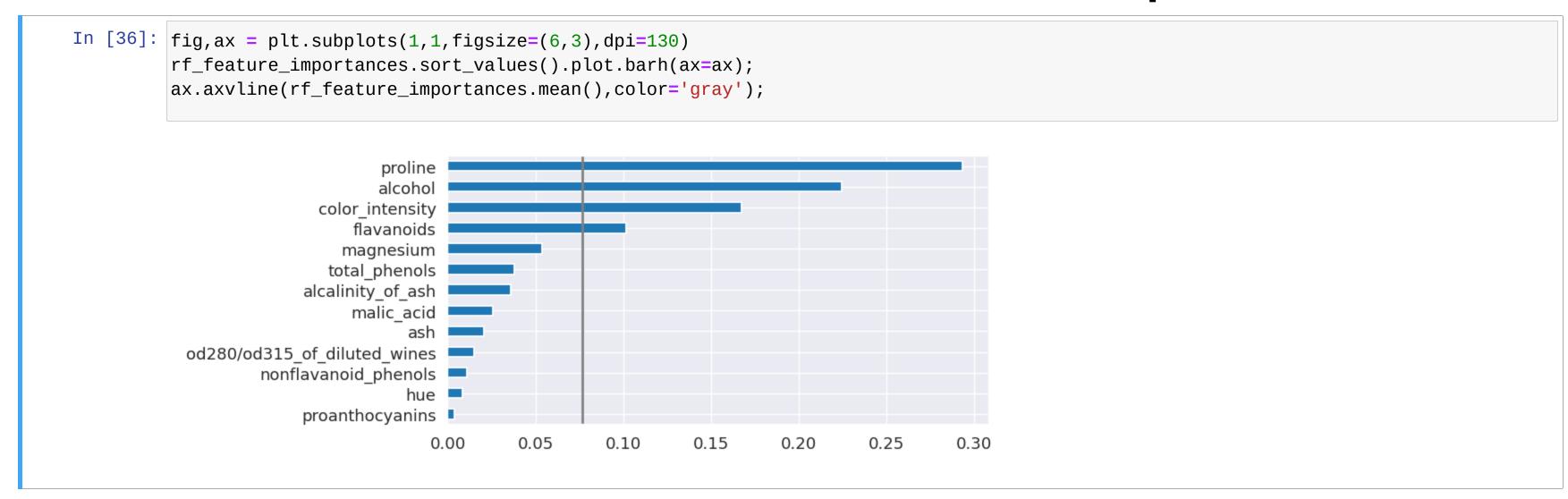
```
In [32]: # Now with LASSO
         logr_l1 = LogisticRegression(C=0.1, penalty="l1", solver="liblinear", random_state=0)
         logr_l1.fit(X_train_zscore, y_train)
         pd.Series(logr_l1.coef_[0],index=wine_feature_names).sort_values(ascending=False).round(5)
Out[32]: malic acid
                                          0.00000
                                         0.00000
         ash
         alcalinity_of_ash
                                         0.00000
         magnesium
                                         0.00000
         total_phenols
                                         0.00000
         flavanoids
                                         0.00000
         nonflavanoid phenols
                                         0.00000
         proanthocyanins
                                         0.00000
         color_intensity
                                         0.00000
                                         0.00000
         hue
         od280/od315 of diluted wines
                                         0.00000
         alcohol
                                         -0.66710
         proline
                                         -1.37284
         dtype: float64
In [33]: # which columns were kept?
         wine_feature_names[logr_l1.coef_[0] != 0]
Out[33]: array(['alcohol', 'proline'], dtype=object)
```

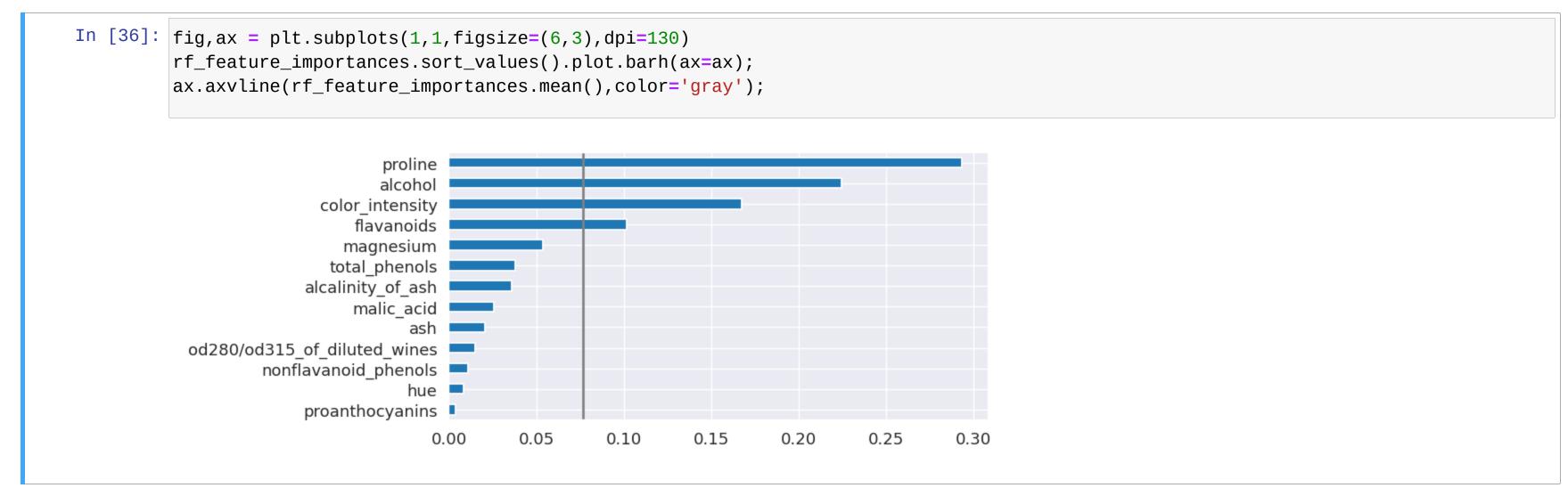
- Trees choose questions based on removing impurity
- We can rank the feature based on how much impurity they remove

- Trees choose questions based on removing impurity
- We can rank the feature based on how much impurity they remove

- Trees choose questions based on removing impurity
- We can rank the feature based on how much impurity they remove

```
In [34]: from sklearn.ensemble import RandomForestClassifier
         rf = RandomForestClassifier(random_state=0).fit(X_train_zscore,y_train)
         rf.feature_importances_.round(3) # (normalized) total reduction of function measuring impurity
Out[34]: array([0.225, 0.026, 0.021, 0.036, 0.054, 0.038, 0.102, 0.011, 0.004,
                0.167, 0.008, 0.015, 0.293])
In [35]: rf_feature_importances = pd.Series(rf.feature_importances_,index=wine_feature_names)
         rf feature importances.sort values(ascending=False).round(3)
Out[35]: proline
                                          0.293
                                          0.225
         alcohol
         color_intensity
                                          0.167
         flavanoids
                                          0.102
         magnesium
                                          0.054
         total_phenols
                                          0.038
         alcalinity_of_ash
                                          0.036
                                          0.026
         malic acid
                                          0.021
         ash
         od280/od315_of_diluted_wines
                                          0.015
         nonflavanoid_phenols
                                          0.011
                                          0.008
         hue
         proanthocyanins
                                          0.004
         dtype: float64
```





- Which of these features should we keep?
 - Elbow method
 - Threshold at mean

```
In [37]: from sklearn.feature_selection import SelectFromModel
         sfm_lr = SelectFromModel(logr_l1,
                                 threshold=None, # if model uses l1 regularization: abs val > 1e-5, otherwise mean
                                                 # don't need to refit, but may give warnings about missing feature manes
                                 prefit=True,
         sfm_lr.get_support() # boolean mask of features selected
Out[37]: array([ True, False, False, False, False, False, False, False,
                False, False, True])
In [38]: wine_feature_names[sfm_lr.get_support()]
Out[38]: array(['alcohol', 'proline'], dtype=object)
In [39]: X_train_subset = sfm_lr.transform(X_train_zscore)
        X_train_subset.shape
         /home/bgibson/anaconda3/envs/eods-f22/lib/python3.10/site-packages/sklearn/base.py:443: UserWarning: X has feature names, but S
         electFromModel was fitted without feature names
           warnings.warn(
Out[39]: (97, 2)
```

```
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                                 threshold=None, # if model uses l1 regularization: abs val > 1e-5, otherwise mean
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                                 prefit=True,
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Out[37]: array([ True, False, False, False, False, False, False, False,
                False, False, True])
In [38]: wine_feature_names[sfm_lr.get_support()]
Out[38]: array(['alcohol', 'proline'], dtype=object)
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         /home/bgibson/anaconda3/envs/eods-f22/lib/python3.10/site-packages/sklearn/base.py:443: UserWarning: X has feature names, but S
         electFromModel was fitted without feature names
           warnings.warn(
Out[39]: (97, 2)
In [40]: X_train_subset[:3].round(3) # note that this is no longer a dataframe
Out[40]: array([[-0.903, -0.853],
                [-1.58, -0.936],
                 [ 0.871, 1.334]])
```

```
In [41]: sfm_rf = SelectFromModel(RandomForestClassifier(),
                                  threshold='mean', # return all features with value greater than the mean (default)
                                  prefit=False
                                                     # will refit (default)
                                 ).fit(X_train_zscore,y_train)
         wine_feature_names[sfm_rf.get_support()]
Out[41]: array(['alcohol', 'magnesium', 'flavanoids', 'color_intensity', 'proline'],
               dtype=object)
In [42]: sfm_rf.estimator_.feature_importances_.mean().round(3)
Out[42]: 0.077
In [43]: |sfm_rf_feature_importances = pd.Series(sfm_rf.estimator_.feature_importances_,index=wine_feature_names)
         sfm_rf_feature_importances.sort_values(ascending=False).round(3)
Out[43]: alcohol
                                         0.266
         proline
                                         0.263
         color intensity
                                         0.114
         flavanoids
                                         0.090
         magnesium
                                         0.079
         total phenols
                                         0.058
         alcalinity_of_ash
                                         0.035
         malic acid
                                         0.023
         ash
                                         0.019
         proanthocyanins
                                         0.016
                                         0.015
         hue
         od280/od315 of diluted wines
                                         0.014
         nonflavanoid_phenols
                                         0.008
         dtype: float64
```

Feature Selection: Univariate Tests

- Perform statistical test on each feature independent of all others
 - Rank and select top k features
 - sklearn: SelectKBest
 - requires a scoring function
- Example: f_classif
 - F-test
 - estimates the degree of linear dependency between feature x and target y

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Feature Selection: Recursive Feature Elimination

- Would like to test all possible combinations of features
- Likely prohibitively expensive/time-consuming
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Feature Selection: Other Methods

- by Variance
 - eliminate columns where all rows have the same (or almost all the same) value
- Sequential Feature Selection
 - greedy algorithm similar to Recursive Feature Elimination
 - uses performance metric (eg accuracy) instead of weights, importances
 - via mlxtend
- Exaustive Feature Selection
 - evaluate all possible feature combinations
 - uses performance metric (eg accuracy) instead of weights, importances
 - via mlxtend
- Other Univariate tests
 - f_regression, F-test for regression task
 - mutual_info_classif and _regression
 - chi2, for classification, requires non-negative values

Questions on Feature Selection?

- Adding features guarantees an increase in ${\it R}^2$
- \mathbb{R}^2 describes the proportion of explained variance
- Additional features explain more variance

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• where n is the number of observations, m is the number of features

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- ${\it R}^2$ describes the proportion of explained variance
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$$R_{adj}^2 = 1 - (1 - R^2) \frac{n - 1}{n - m - 1}$$

• where *n* is the number of observations, *m* is the number of features

```
In [46]: def adj_r2(model,X,y):
    n,m = X.shape
    return 1-(1-model.score(X,y))*(n-1)/(n-m-1)
```

```
In [47]: from sklearn.linear_model import LinearRegression

X_r = X_train_zscore.loc[:,wine_feature_names != 'alcohol'] # get all features except alchohol
y_r = X_train_zscore.loc[:,'alcohol'] # predict alcohol from other features

lr = LinearRegression()
print('R2 with 3 features :', lr.fit(X_r.iloc[:,:3],y_r).score(X_r.iloc[:,:3],y_r).round(2))
print('R2 with all features :', lr.fit(X_r.iloc[:,:],y_r).score(X_r.iloc[:,:],y_r).round(2))

R2 with 3 features : 0.37
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```

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Adj R2 with 3 features : 0.35
Adj R2 with all features : 0.62
```

• Now we know the increase is due to a better model and not just adding features

```
In [49]: from statsmodels.api import OLS
          model = OLS(y_r, X_r).fit()
          print(model.rsquared_adj.round(3))
          model.summary()
          0.621
Out[49]:
          OLS Regression Results
           Dep. Variable:
                                         R-squared (uncentered):
                                                               0.668
                          alcohol
```

Model:	OLS	Adj. R-squared (uncentered):	0.621
Method:	Least Squares	F-statistic:	14.23
Date:	Wed, 02 Nov 2022	Prob (F-statistic):	1.06e-15
Time:	17:21:35	Log-Likelihood:	-84.207
No. Observations:	97	AIC:	192.4
Df Residuals:	85	BIC:	223.3
Df Model:	12		
Covariance Type:	nonrobust		

		std err	t	P> t	[0.025	0.975]
malic_acid	0.1823	0.074	2.449	0.016	0.034	0.330
ash	-0.0314	0.104	-0.302	0.764	-0.238	0.175
alcalinity_of_ash	-0.1651	0.097	-1.706	0.092	-0.357	0.027
magnesium	0.0060	0.077	0.079	0.937	-0.146	0.158
total_phenols	0.0701	0.126	0.555	0.580	-0.181	0.321
flavanoids	0.0260	0.183	0.142	0.888	-0.338	0.390
nonflavanoid_phenols	0.0545	0.086	0.631	0.530	-0.117	0.226
proanthocyanins	-0.1407	0.082	-1.717	0.090	-0.304	0.022
color_intensity	0.3190	0.138	2.316	0.023	0.045	0.593
hue	0.1609	0.074	2.183	0.032	0.014	0.308

Questions re Adjusted \mathbb{R}^2 ?

Feature Extraction

- Transform original features into new feature space
- Can be thought of as compression while maintaining relevant information
- Often used for:
 - visualization (multi-dimensional to 2-D)
 - compression (storage)
 - dimensionality reduction
- Popular methods:
 - Principal Component Analysis: Unsupervised data compression
 - Linear Discriminant Analysis: Supervised method to maximize class separation
 - Kernel PCA, etc.

Principal Component Analysis (PCA)

- Unsupervised Learning method (ignores label)
- Idea:
 - Directions of high variance in the data contain important information
 - Colinear features can be combined
 - Find directions of maximum variance
 - Project onto subspace with same or fewer dimensions

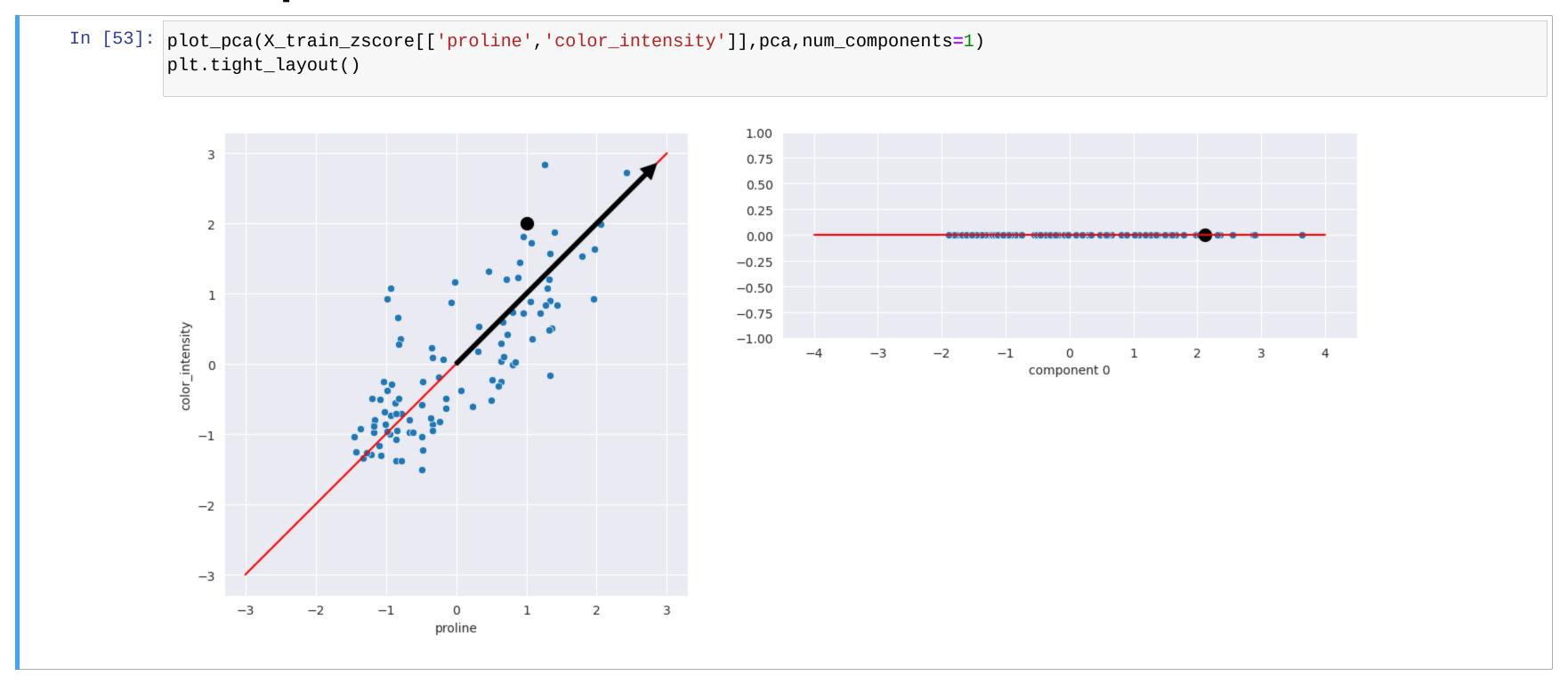
Principal Component Analysis (PCA)

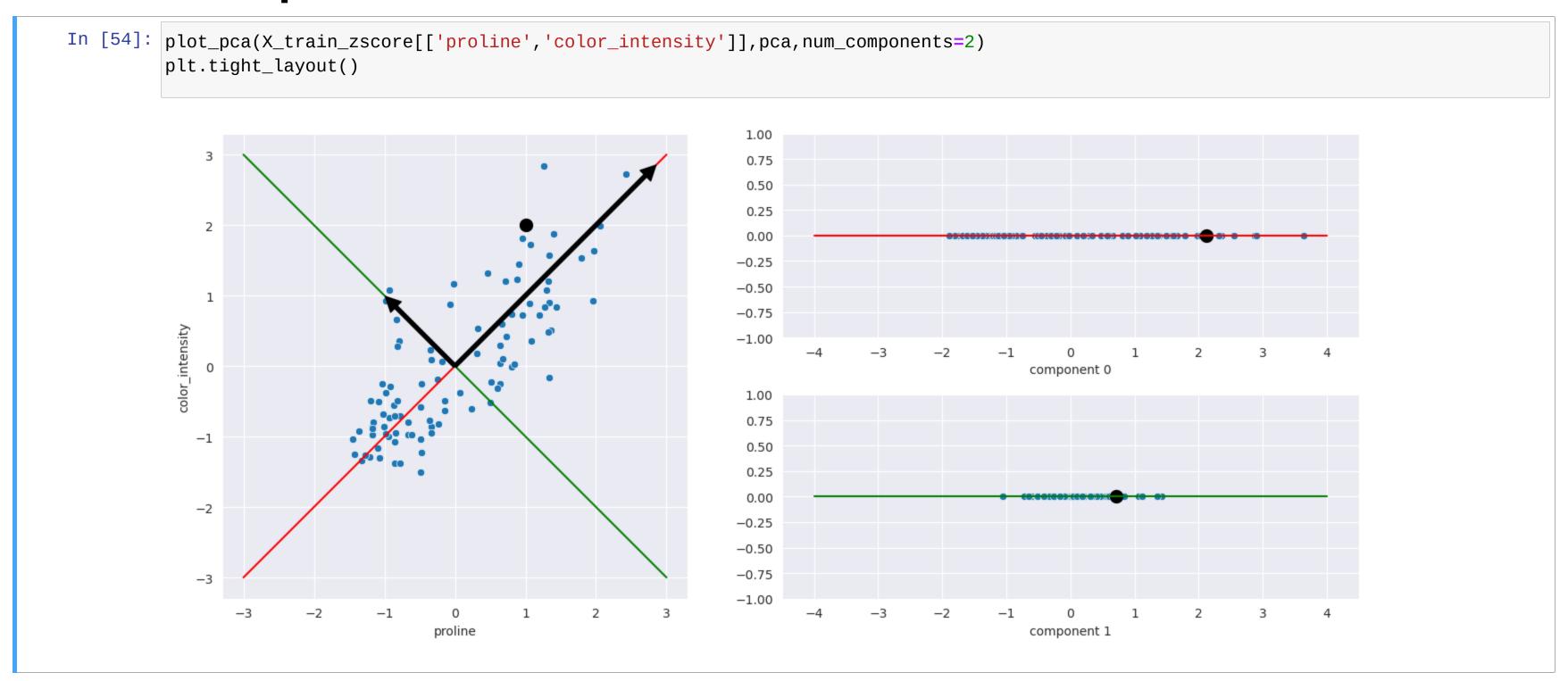
- How it works:
 - O. first center the data (subtract the means)
 - 1. extract first component:
 - direction (combination of features)
 - explains maximum variance
 - 2. extract next component:
 - direction, orthogonal to the first (linearly independent)
 - explains max remaining variance
 - 3. repeat:
 - max number of possible components equals number of original dimensions

PCA Example

PCA Example

```
In [51]: fig,ax = plt.subplots(1,1,figsize=(8,8))
          sns.scatterplot(x='proline',y='color_intensity',data=X_train_zscore,ax=ax);
           color_intensity
                 -1.5
                                                    1.0
                                                          1.5
                                                                 2.0
                                            proline
```





PCA in sklearn

PCA in sklearn

PCA in sklearn

```
In [55]: from sklearn.decomposition import PCA
         pca = PCA().fit(X_train_zscore)
         print(f'num input features: {X_train_zscore.shape[1]}')
         print(f'num pca components: {pca.n_components_}')
         num input features: 13
         num pca components: 13
In [56]: pca.components_[0].round(2)
Out[56]: array([ 0.35, -0.05,  0.16, -0.18,  0.23,  0.38,  0.4 , -0.22,  0.24,
                 0.38, 0.12, 0.21, 0.39])
In [57]: print(' + \n'.join([f'{w: 0.2f}*{f}' for f,w in zip(wine_feature_names,pca.components_[0])])
          0.35*alcohol +
         -0.05*malic acid +
          0.16*ash +
         -0.18*alcalinity_of_ash +
          0.23*magnesium +
          0.38*total_phenols +
          0.40*flavanoids +
         -0.22*nonflavanoid phenols +
          0.24*proanthocyanins +
          0.38*color_intensity +
          0.12*hue +
          0.21*od280/od315 of diluted wines +
          0.39*proline
```

PCA: Explained Variance

• How much of the variance in the dataset is explained by each component?

PCA: Explained Variance

component

• How much of the variance in the dataset is explained by each component?

```
In [58]: pca = PCA().fit(X_train_zscore)
         print(f'explained_variance
                                        : {pca.explained_variance_.round(2)}')
         print(f'explained_variance_ratio_ : {pca.explained_variance_ratio_.round(2)}')
         print(f'cumulative explained variance : {pca.explained_variance_ratio_.cumsum().round(2)}')
         df_var = pd.DataFrame({'component':range(pca.n_components_),
                                 'cumulative explained variance':pca.explained_variance_ratio_.cumsum()})
         sns.pointplot(x='component',y='cumulative explained variance',data=df_var);
         explained_variance
                                        : [4.75 1.96 1.56 1.22 0.84 0.74 0.59 0.42 0.33 0.26 0.22 0.17 0.07]
         explained_variance_ratio_ : [0.36 0.15 0.12 0.09 0.06 0.06 0.05 0.03 0.03 0.02 0.02 0.01 0.01]
         cumulative explained variance: [0.36 0.51 0.63 0.72 0.79 0.84 0.89 0.92 0.95 0.97 0.98 0.99 1. ]
            1.0
            0.9
          cumulative explained variance
            0.7
            0.6
            0.5
            0.4
```

Dimensionality Reduction with PCA

Dimensionality Reduction with PCA

```
In [59]: pca_2d = PCA(n_components=2)
         X_pca = pca_2d.fit_transform(X_train_zscore)
         X_pca = pd.DataFrame(X_pca,columns=['component0','component1'])
          fig, ax=plt.subplots(1,2,figsize=(14,6))
          sns.scatterplot(x='proline',y='color_intensity',data=X_train_zscore,ax=ax[0]);
          sns.scatterplot(x='component0',y='component1',data=X_pca,ax=ax[1]);
          ax[0].axis('equal');ax[1].axis('equal');
           color_intensity
                                                                component1
             -1
               -2
                                                                                                 2
                                    proline
                                                                                       component0
```

Image Recognition Example

PCA and Image Recognition

- Generally, an image is represented by a grid of pixels
- Each pixel is a square that takes a value representing a shade (usually a value between 0 and 255)
- 1024 x 1024 pixels = 1,048,576 pixels = 1 megapixel
- iPhone X11 Pro: 12 megapixels
- Color images contain three layers: red, green, blue
- ~36 million pixel values
- A very high dimensional space!

- Image classification using PCA?
 - Example based on <u>Faces recognition example using eigenfaces and SVMs</u>

Example Dataset: Labeled Faces in th Wild (LFW)

Labeled Faces in the Wild

Example Dataset: Labeled Faces in th Wild (LFW)

Labeled Faces in the Wild

```
In [60]: from sklearn.datasets import fetch_lfw_people
lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.6)
```

Example Dataset: Labeled Faces in th Wild (LFW)

Labeled Faces in the Wild

```
In [60]: from sklearn.datasets import fetch_lfw_people
         lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.6)
In [61]: sns.set_style('dark')
         plt.imshow(lfw_people.images[1], cmap=plt.cm.gray, vmin=0, vmax=1)
         plt.title(lfw_people.target_names[lfw_people.target[1]], size=12);
                     Tony Blair
          20
          50
```

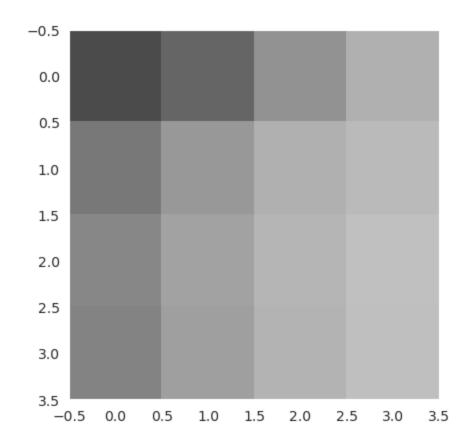
Example Pixel Values

Example Pixel Values



Example Pixel Values

```
In [62]: # sample of 3x3 set of pixels
plt.imshow(lfw_people.images[1][20:24,20:24],cmap=plt.cm.gray,vmin=0, vmax=1);
```



```
In [64]: lfw_people.images[1].shape
Out[64]: (75, 56)
```

• Grid as a fixed length feature vector?

What information do we lose when we do this?

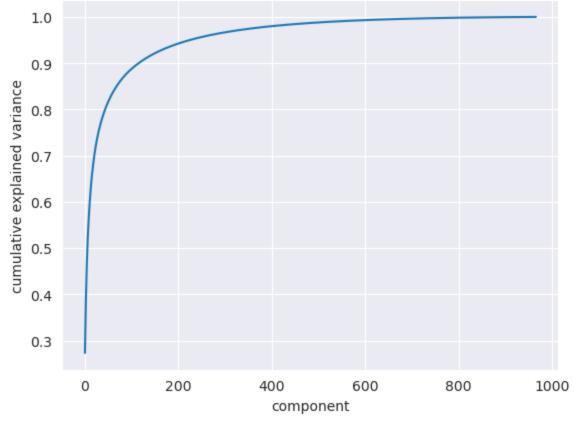
Create a Dataset

Create a Dataset

```
In [67]: # get the shape of images for plotting the
         n_samples, h, w = lfw_people.images.shape
         # use actual pixel values, ignoring relative position
        X_faces = lfw_people.data
         n_features = X_faces.shape[1]
         # the label to predict is the id of the person
         y_faces = lfw_people.target
         target_names = lfw_people.target_names
         n_classes = target_names.shape[0]
         # create train/test split
        X_train_faces, X_test_faces, y_train_faces, y_test_faces = train_test_split(X_faces, y_faces,
                                                                                    test_size=0.25,
                                                                                    stratify=y_faces,
                                                                                    random_state=0)
         print(f"image_size: {h}x{w}")
         print("n_features: %d" % n_features)
         print("n_classes : %d" % n_classes)
         print(f"n_train : {len(X_train_faces)}")
         print(f"n_test : {len(X_test_faces)}")
         image_size: 75x56
         n features: 4200
         n_classes : 7
         n train : 966
         n_test : 322
```

Variance explained by PCA

Variance explained by PCA



```
In [69]: # set the number of dimensions we want to retain
        n_{components} = 200
        # instantiate and fit on X train
        pca_faces = PCA(n_components=n_components,
                       svd_solver='randomized',
                       whiten=True).fit(X_train_faces)
        # extract and reshape components into eigenfaces for plotting
        eigenfaces = pca_faces.components_.reshape((n_components, h, w))
        # transform the training and test set for classification
        X_train_faces_pca = pca_faces.transform(X_train_faces)
        X_test_faces_pca = pca_faces.transform(X_test_faces)
In [70]: pca_faces.components_[0].round(2)
Out[70]: array([0.01, 0.01, 0.01, ..., 0. , 0. , 0. ], dtype=float32)
In [71]: pca_faces.singular_values_.round(2)
Out[71]: array([255.19, 117.42, 115.07, 102.78, 91.69, 84.31, 79.27, 70.63,
                66.71, 65.5 , 61.31, 58.95, 56.8 ,
                                                      54.46,
                                                             52.38,
                                                                     49.04,
                46.8 , 45.43, 44.75, 44.01, 42.64,
                                                      41.01,
                                                             40.44, 38.07,
                                                      32.88,
                37.74, 35.97, 35.33, 34.61,
                                              33.79,
                                                              32.09,
                                                                     31.6 ,
                31.08, 30.14, 29.7, 29.02,
                                              28.72,
                                                      28.21,
                                                             27.53,
                                                                     27.3 ,
                26.96, 26.69, 26.44, 25.95,
                                              25.12, 24.88,
                                                             24.59,
                                                                     24.34,
                23.93, 23.57, 23.37, 22.91, 22.77, 22.53, 22.44, 22.16,
                21.83, 21.69, 21.26, 21.01, 20.87, 20.6,
                                                             20.48,
                                                                     20.2 ,
                19.92, 19.8, 19.59, 19.23, 19.12, 18.93, 18.78, 18.67,
                18.51, 18.24, 18.16, 18.05, 17.9, 17.74, 17.57, 17.47,
                17.33, 17.03, 16.83, 16.61, 16.52, 16.32, 16.26, 16.15,
                16 05 15 04 15 60 15 67 15 50 15 45 15 20 15 12
```

```
In [72]: def plot_gallery(images, titles, h, w, n_row=3, n_col=4):
            """Helper function to plot a gallery of portraits"""
            plt.figure(figsize=(1.8 * n_col, 2.4 * n_row))
            plt.subplots_adjust(bottom=0, left=.01, right=.99, top=.90, hspace=.35)
            for i in range(n_row * n_col):
               plt.subplot(n_row, n_col, i + 1)
               plt.imshow(images[i].reshape((h, w)), cmap=plt.cm.gray)
               plt.title(titles[i], size=12)
               plt.xticks(())
               plt.yticks(())
            plt.tight_layout()
        # plot the result of the prediction on a portion of the test set
        def title(y_pred, y_test, target_names, i):
            pred_name = target_names[y_pred[i]].rsplit(' ', 1)[-1]
            true_name = target_names[y_test[i]].rsplit(' ', 1)[-1]
```



Train and Tune SVC

Train and Tune SVC

Train and Tune SVC

Evaluate on the test set

Evaluate on the test set

```
In [76]: from sklearn.metrics import classification_report
         y_pred_pca = clf_faces_pca.predict(X_test_faces_pca)
         print(classification_report(y_test_faces, y_pred_pca, target_names=target_names))
                            precision
                                                            support
                                         recall f1-score
              Ariel Sharon
                                 0.65
                                           0.58
                                                     0.61
                                                                 19
                                                     0.74
              Colin Powell
                                 0.74
                                           0.73
                                                                 59
           Donald Rumsfeld
                                 0.76
                                                     0.69
                                                                 30
                                           0.63
                                 0.80
                                           0.91
                                                     0.85
                                                                133
             George W Bush
         Gerhard Schroeder
                                 0.77
                                           0.63
                                                     0.69
                                                                 27
               Hugo Chavez
                                                                 18
                                 0.64
                                           0.50
                                                     0.56
                Tony Blair
                                 0.77
                                           0.75
                                                     0.76
                                                                 36
                                                     0.77
                                                                322
                  accuracy
                                 0.73
                                                     0.70
                                                                322
                 macro avg
                                           0.68
              weighted avg
                                 0.76
                                           0.77
                                                     0.76
                                                                322
```

Prediction Examples

Prediction Examples

```
In [77]: prediction_titles = [title(y_pred_pca, y_test_faces, target_names, i)
                                for i in range(y_pred_pca.shape[0])]
          plot_gallery(X_test_faces[10:], prediction_titles[10:], h, w)
          plt.tight_layout()
           predicted: Bush
                          predicted: Bush
                                         predicted: Blair predicted: Schroeder
            true: Bush
                                          true: Blair
                                                               Blair
                                                         true:
```

predicted: Bush Bush

predicted: Powell predicted: Rumsfeld predicted: Bush true: Powell true: Rumsfeld





true: Bush



predicted: Powell true: Powell



true: Bush



true: Blair



predicted: Bush predicted: Schroeder predicted: Bush true: Bush









Performance without PCA: Train

Performance without PCA: Train

```
%%time
# Warning: this cell takes up to 3 minutes to execute on an Intel i7 1.8Ghz w/ 8 cores
params = \{'C': [1e3, 5e3, 1e4, 5e4, 1e5],
          'gamma': [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.1],}
clf_faces_nopca = GridSearchCV(SVC(kernel='rbf', class_weight='balanced'),
                                   params, cv=3, n_jobs=-1)
clf_faces_nopca = clf_faces_nopca.fit(X_train_faces, y_train_faces)
#CPU times: user 2.08 s, sys: 53.3 ms, total: 2.13 s
#Wall time: 2min 42s
print(f"best_params : {clf_faces_nopca.best_params_}")
print(f"best_score : {clf_faces_nopca.best_score_:0.2f}")
#best_params : {'C': 1000.0, 'gamma': 0.0001}
#best_score : 0.78
```

Performance without PCA: Evaluate

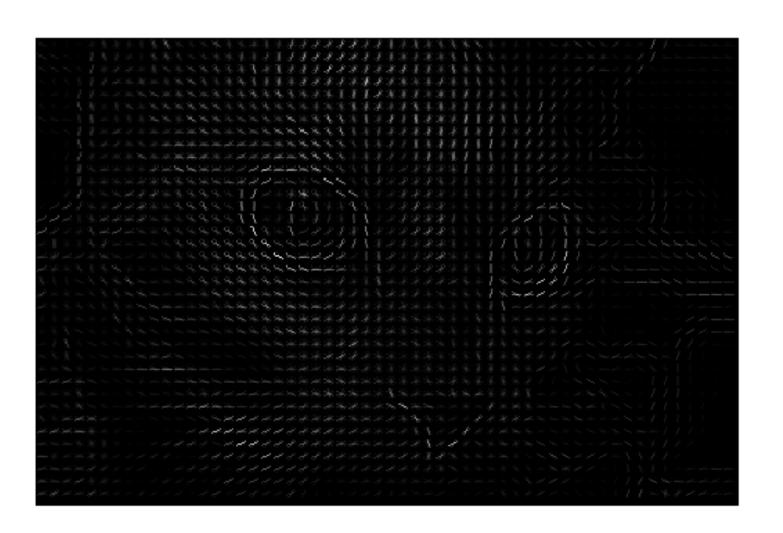
Performance without PCA: Evaluate

```
y_pred_nopca = clf_faces_nopca.predict(X_test_faces)
print(classification_report(y_test_faces, y_pred_nopca, target_names=target_names))
                    precision
                                recall f1-score
#
                                                    support
      Ariel Sharon
                         0.65
                                   0.79
                                             0.71
                                                         19
      Colin Powell
                         0.82
                                   0.69
                                             0.75
                                                         59
    Donald Rumsfeld
                                   0.60
                                             0.60
                         0.60
                                                         30
     George W Bush
                                   0.90
                         0.82
                                             0.86
                                                        133
 Gerhard Schroeder
                         0.56
                                   0.56
                                             0.56
                                                         27
#
       Hugo Chavez
                         0.71
                                   0.28
                                             0.40
                                                         18
        Tony Blair
                         0.71
                                   0.75
                                             0.73
                                                         36
                                                        322
                                             0.75
          accuracy
#
                                   0.65
                                             0.66
                         0.70
                                                        322
         macro avg
      weighted avg
                                                        322
                         0.75
                                   0.75
                                             0.74
```

Other Image Recognition Methods

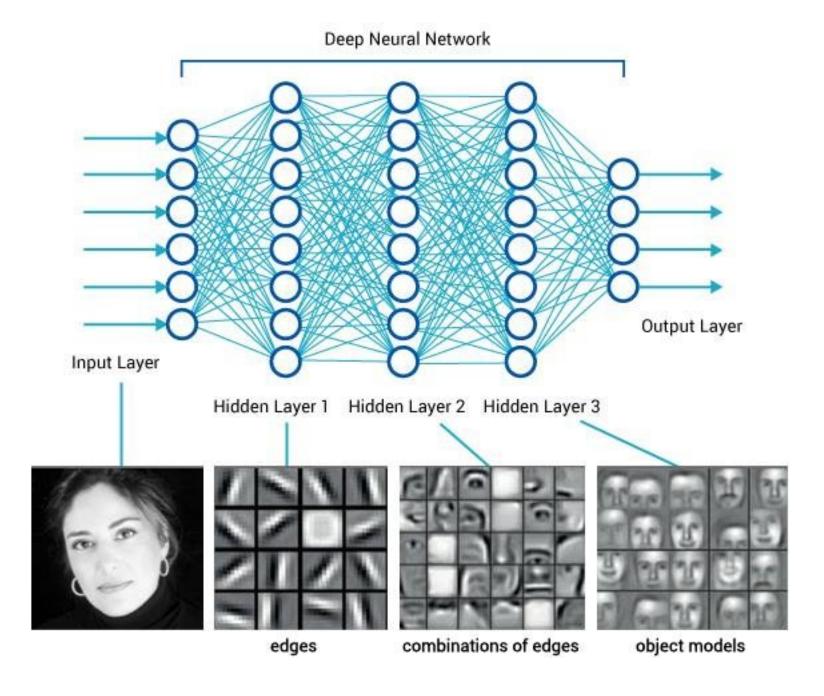
- With Feature Engineering and general models
 - ex: Histogram of Oriented Gradients or HOG (See <u>PDSH Chap 5</u>)
 - many more (See <u>scikit-image</u>)





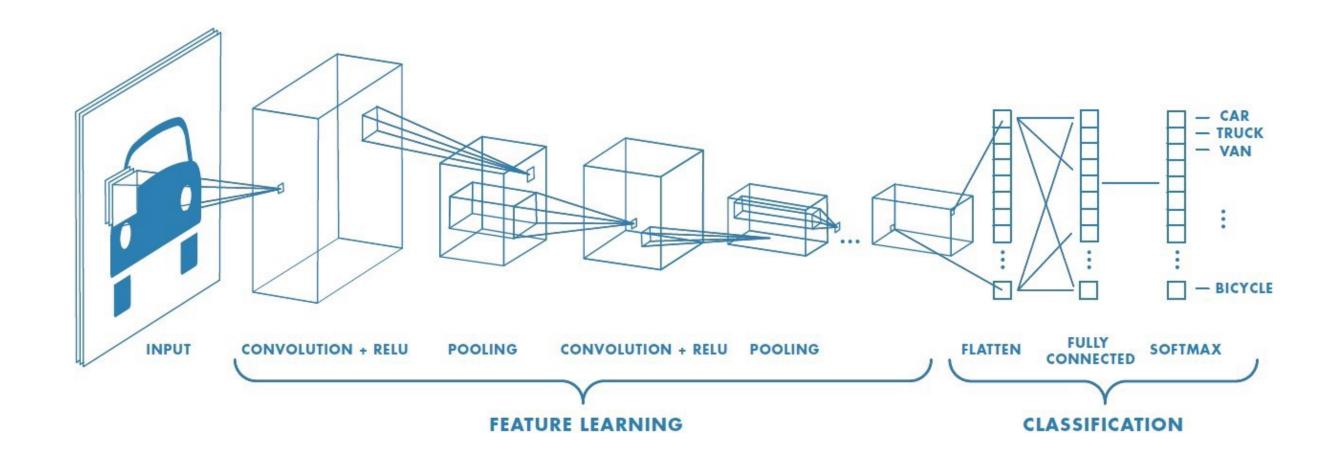
Other Image Recognition Methods: Deep Neural Networks

With Deep Neural Nets



Other Image Recognition Methods: Deep Neural Networks

• With Convolutional Neural Networks <u>Good Example</u>



Questions re Feature Extraction and PCA?

Next time: NLP and Pipelines