#### Elements Of Data Science - F2024

# Week 9: Dimensionality Reduction, Feature Selection and Feature Extraction

11/18/2024

#### **TODOs**

- Readings:
  - PML Chapter 6.1, Streamlining workflows with Pipelines
  - PML Chapter 8: Applying Machine Learning to Sentiment Analysis
- HW 3, Due Mon Dec 2nd, 11:59pm ET

### **Today**

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

Questions?

# **Environment Setup**

# **Environment Setup**

```
In [1]: 1 import numpy
2 import numpy as np
3 import pandas as pd
4 import matplotlib.pyplot as plt
5 import seaborn as sns
6
7 from mlxtend.plotting import plot_decision_regions
8
9 sns.set_style('darkgrid')
10 %matplotlib inline
```

# Joing Datasets

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

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### 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

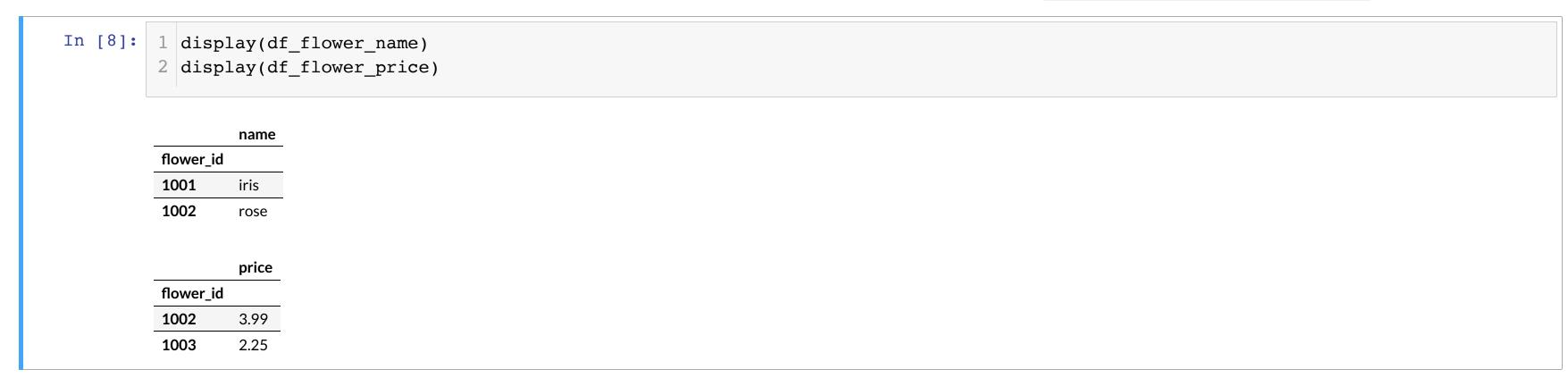
- easiest way to join Pandas DataFrames is on row index label
- may need to set the index from a column using .set\_index()

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

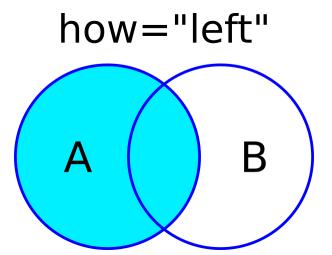


```
In [8]: 1 display(df_flower_name)
         2 display(df_flower_price)
                  name
          flower_id
                  iris
          1001
          1002
                  rose
                  price
          flower id
                  3.99
          1002
                  2.25
          1003
In [9]: 1 df_flower_name.join(df_flower_price)
         2 # df_flower_price.join(df_flower_name)
Out[9]:
                  name price
          flower_id
          1001
                       NaN
                  iris
          1002
                  rose
                       3.99
```

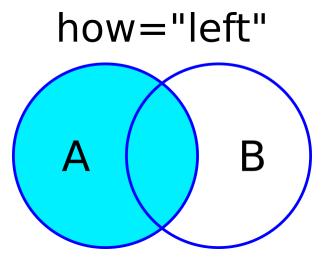
```
In [8]: 1 display(df_flower_name)
          2 display(df_flower_price)
                  name
          flower_id
                  iris
          1001
          1002
                  rose
                  price
          flower id
                  3.99
          1002
                  2.25
          1003
In [9]: 1 df_flower_name.join(df_flower_price)
          2 # df flower price.join(df flower name)
Out[9]:
                  name price
          flower id
          1001
                        NaN
                  iris
          1002
                        3.99
                  rose
```

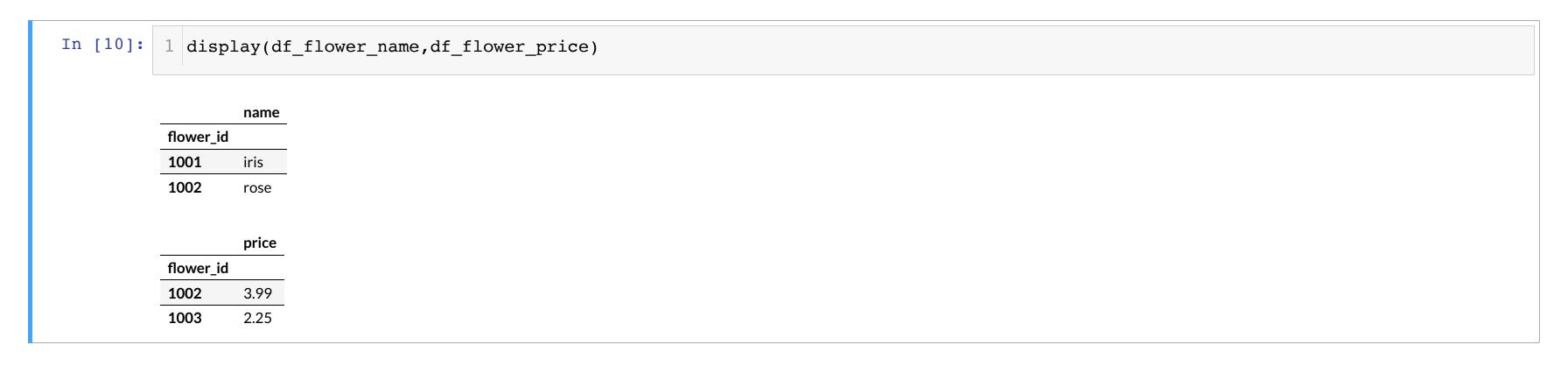
• by default, this is a 'Left Join'

Join Types: Left Join

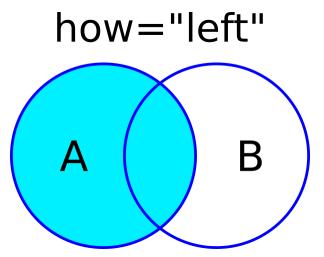


#### Join Types: Left Join





#### Join Types: Left Join



```
In [10]: 1 display(df_flower_name,df_flower_price)
name
```

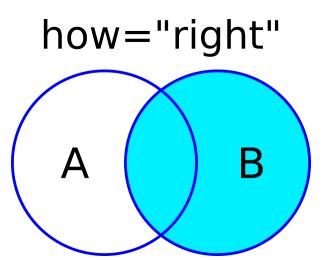
	Hanne
flower_id	
1001	iris
1002	rose

	price
flower_id	
1002	3.99
1003	2.25

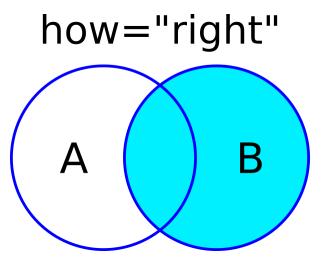
```
In [11]: 1 df_flower_name.join(df_flower_price,how="left") # default for df.join() is left join
Out[11]:
```

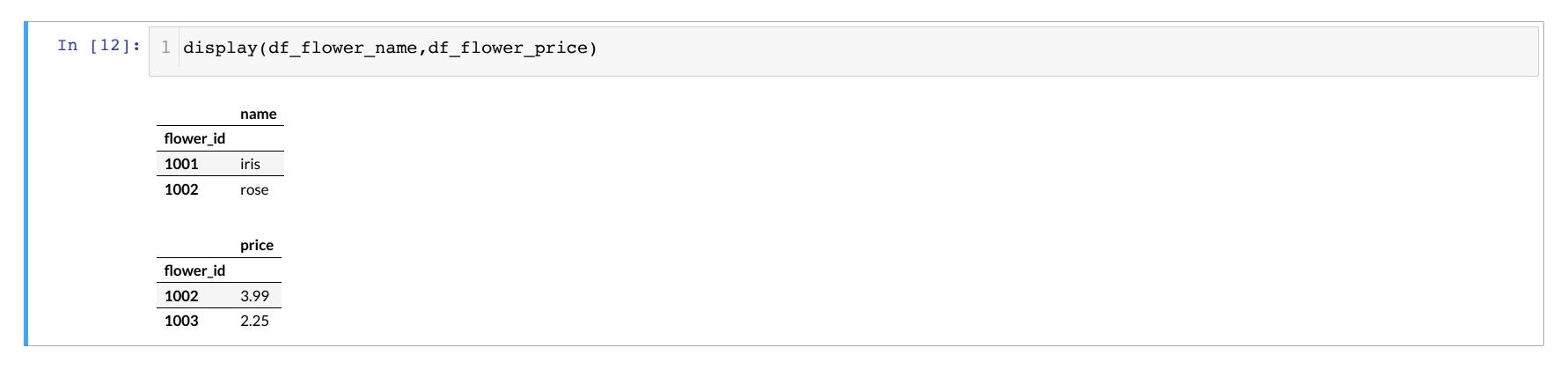
_	name	price
flower_id		
1001	iris	NaN
1002	rose	3.99

Join Types: Right Join

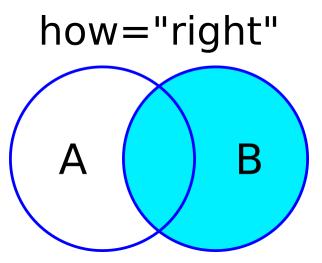


#### Join Types: Right Join



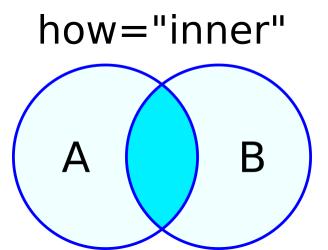


#### Join Types: Right Join

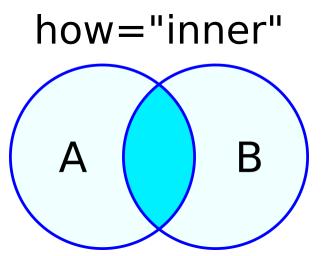


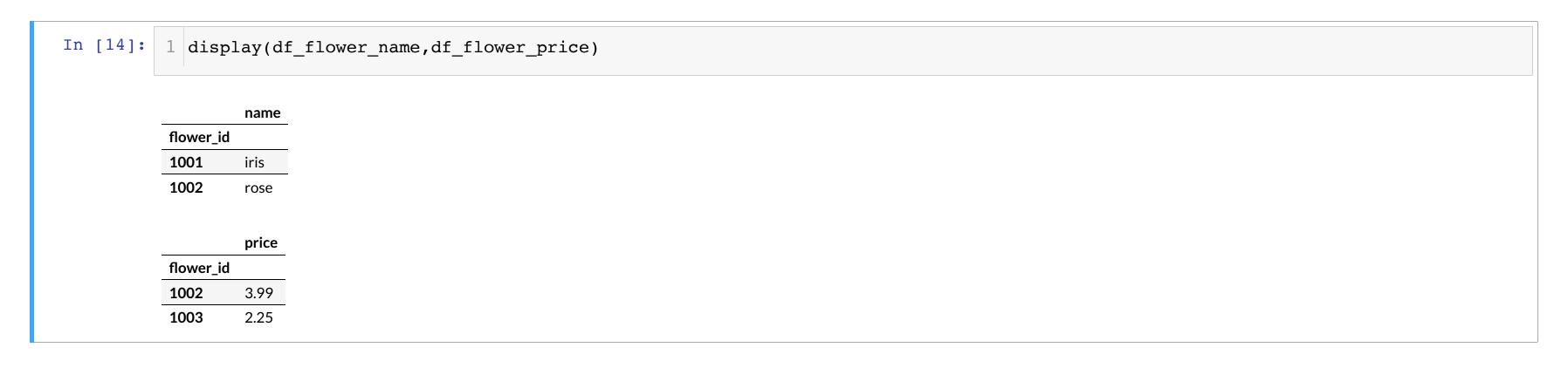
```
In [12]: 1 display(df_flower_name,df_flower_price)
                   name
           flower_id
           1001
                   iris
           1002
                   rose
                   price
           flower_id
           1002
                   3.99
                   2.25
           1003
In [13]: 1 df_flower_name.join(df_flower_price,how='right')
Out[13]:
                   name price
           flower_id
                        3.99
           1002
                   rose
           1003
                   NaN
                        2.25
```

Join Types: Inner Join

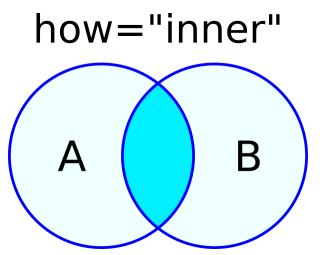


#### Join Types: Inner Join



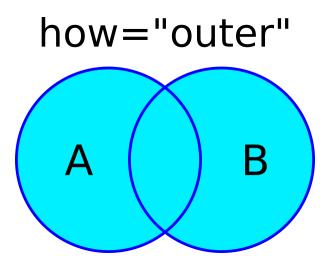


#### Join Types: Inner Join

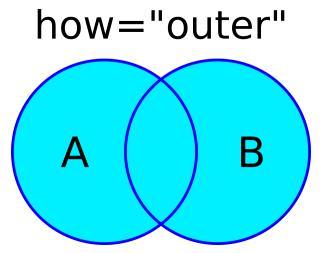


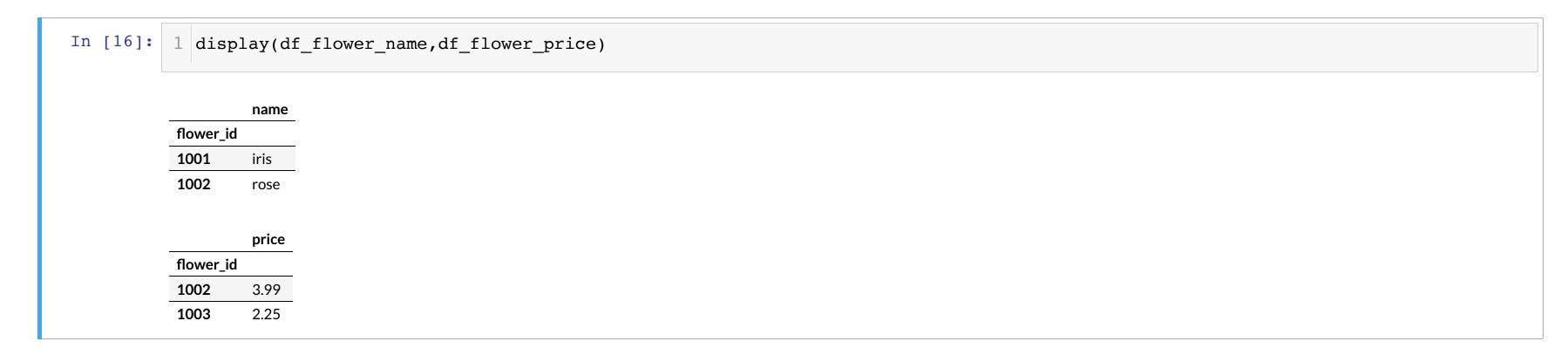
```
In [14]: 1 display(df_flower_name,df_flower_price)
                   name
           flower_id
                   iris
           1001
           1002
                   rose
                   price
           flower_id
           1002
                   3.99
                   2.25
           1003
In [15]: 1 df_flower_name.join(df_flower_price,how='inner')
Out[15]:
                   name price
           flower_id
           1002
                   rose 3.99
```

Join Types: Outer Join



#### Join Types: Outer Join

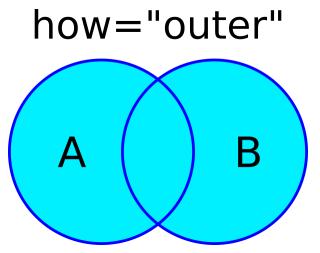




#### Join Types: Outer Join

1003

NaN 2.25



```
In [16]: 1 display(df_flower_name,df_flower_price)
                   name
           flower_id
                   iris
           1001
           1002
                   rose
                   price
           flower_id
           1002
                   3.99
                   2.25
           1003
In [17]: 1 df_flower_name.join(df_flower_price,how='outer')
Out[17]:
                   name price
           flower_id
                   iris
           1001
                        NaN
                        3.99
           1002
                   rose
```

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

```
In [20]: 

# imagine that 'name' is a categorical variable

Out[20]: 

name
flower_id
1001 iris
1002 rose
```

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

```
In [20]: 1 # imagine that 'name' is a categorical variable
          2 df_flower_name[['name']]
Out[20]:
                   name
           flower id
                  iris
           1001
           1002
                  rose
In [21]: | 1 # converting categorical to one-hot using get_dummies
          2 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]: 1 # can join back using the default index
          2 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
                  iris 1
           1001
           1002
                  rose 0
```

# 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()

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

```
In [23]: 1 # using the dataframes before setting index using .set_index()
          2 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
          0 1002
                    rose 3.99
In [24]: 1 # if both id columns have the same name, can just use "on="
         2 pd.merge(df flower name orig,
                     df flower price orig,
                     on='flower id',
                     how='outer')
Out[24]:
            flower_id name price
          0 1001
                        NaN
          1 1002
                        3.99
          2 1003
                    NaN 2.25
```

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]:
          1 from sklearn.datasets import load wine
          2 from sklearn.model_selection import train_test_split
          4 wine = load wine()
          6 X_wine = pd.DataFrame(wine.data,columns=wine.feature_names)
          7 y_wine = wine.target
          9 # reduce to binary classification
         10 X wine = X wine.iloc[y wine < 2]
         11 y_wine = y_wine[y_wine < 2]</pre>
         12
         13 X train, X_test, y_train, y_test = train_test_split(X_wine, y_wine, stratify=y_wine, random_state=0)
         14
         15 wine_feature_names = X_wine.columns.values
         16 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

**30** 13.73

1.50

2.70 22.5

101.0

3.00

3.25

```
In [25]:
          1 from sklearn.datasets import load wine
           2 from sklearn.model selection import train test split
           4 wine = load wine()
           6 X wine = pd.DataFrame(wine.data,columns=wine.feature names)
           7 y wine = wine.target
          9 # reduce to binary classification
         10 X wine = X wine.iloc[y wine < 2]
         11 y wine = y wine[y wine < 2]
         12
         13 X train, X test, y train, y test = train test split(X wine, y wine, stratify=y wine, random state=0)
         14
         15 wine feature names = X wine.columns.values
         16 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]: 1 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 proline
                              2.31 22.8
          86 12.16
                     1.61
                                               90.0
                                                        1.78
                                                                   1.69
                                                                           0.43
                                                                                            1.56
                                                                                                         2.45
                                                                                                                    1.33 2.26
                                                                                                                                                495.0
           121 11.56
                     2.05
                              3.23 28.5
                                               119.0
                                                        3.18
                                                                   5.08
                                                                           0.47
                                                                                            1.87
                                                                                                         6.00
                                                                                                                     0.93 3.69
                                                                                                                                                465.0
```

0.29

2.38

5.70

1.19 2.71

1285.0

#### **Need to Standardize Features**

#### **Need to Standardize Features**

]:	mean	std	
alcohol	13.0	0.9	
malic_acid	2.0	0.9	
ash	2.4	0.3	
alcalinity_of_ash	19.1	3.7	
magnesium	99.1	15.0	
total_phenols	2.5	0.5	
flavanoids	2.5	0.8	
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	
proline	803.1	363.2	

## **Standardize Features**

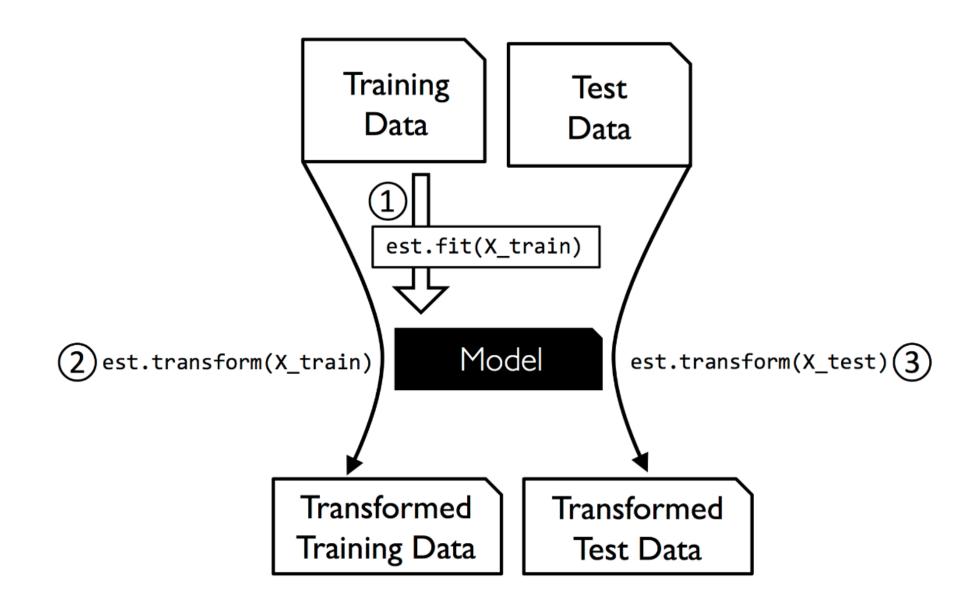
#### **Standardize Features**

#### **Standardize Features**

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

## Recall: Predicting vs Transforming with Train/Test Split

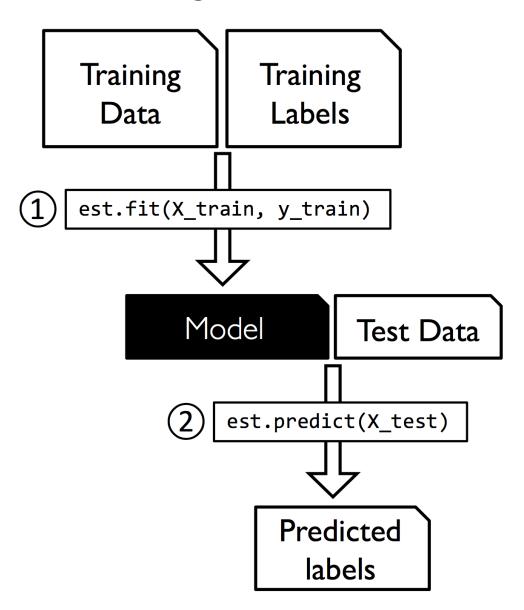
- When transforming data, fit on the training set, transform both train and test



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  $\ell_1$  or 11 regularization drives the coefficient of uninformative features to 0

## Feature Selection: LASSO (L1)

• LASSO or  $\ell_1$  or 11 regularization drives the coefficient of uninformative features to 0

## Feature Selection: LASSO (L1)

• LASSO or  $\ell_1$  or 11 regularization drives the coefficient of uninformative features to 0

```
In [30]: 1 from sklearn.linear model import LogisticRegression
         3 # First, without regularization
         4 logr = LogisticRegression(penalty="none", solver="lbfgs", random_state=0)
         5 logr.fit(X train zscore, y train)
         6 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, -14.431
In [31]: 1 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
                                        -4.41
         malic acid
                                        -8.11
         ash
                                        -8.14
         alcohol
                                       -14.43
         proline
         dtype: float64
```

Feature Selection: LASSO (L1) Cont.

Oracle

#### Feature Selection: LASSO (L1) Cont.

#### Oracle

```
In [32]: 1
          2 # Now with LASSO
                C is the inverse regularization strength: higher means less regularization
         4 logr_l1 = LogisticRegression(C= .1, penalty="l1", solver="liblinear", random_state=0)
         5 logr_l1.fit(X_train_zscore, y_train)
          6
         7 pd.Series(logr_l1.coef_[0],index=wine_feature_names).sort_values(ascending=False).round(5)
Out[32]: malic acid
                                          0.00000
         ash
                                          0.00000
         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.

#### **Oracle**

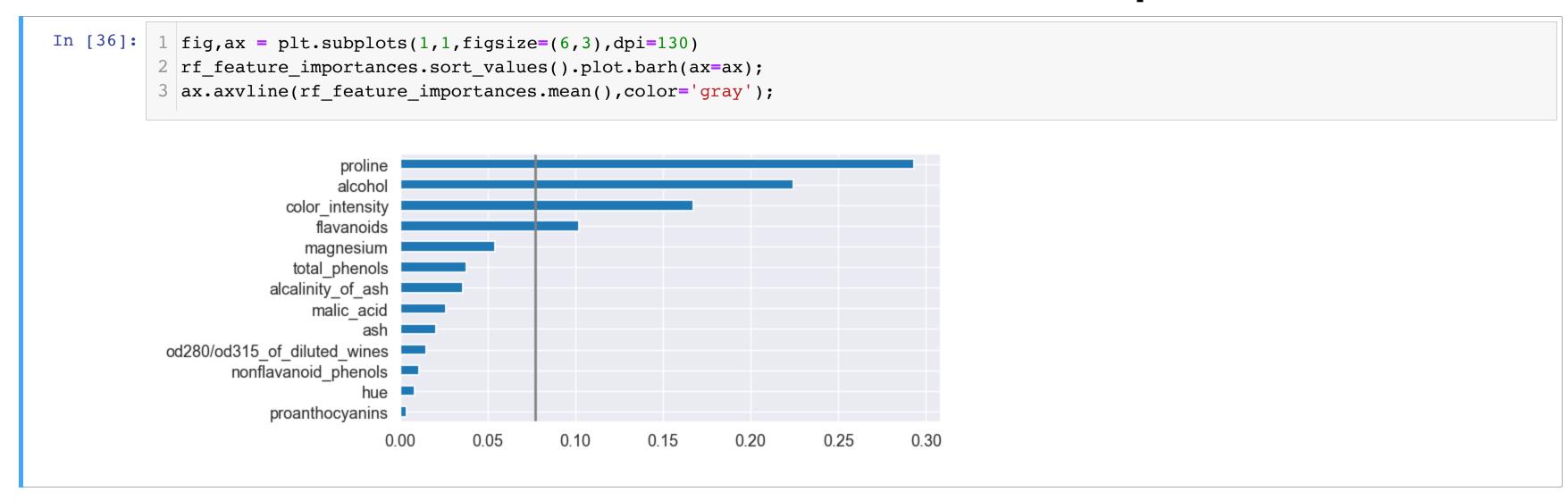
```
In [32]: 1
         2 # Now with LASSO
               C is the inverse regularization strength: higher means less regularization
         4 logr l1 = LogisticRegression(C= .1, penalty="l1", solver="liblinear", random state=0)
         5 logr l1.fit(X train zscore, y train)
          6
         7 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
         hue
                                          0.00000
         od280/od315 of diluted wines
                                          0.00000
                                         -0.66710
         alcohol
         proline
                                         -1.37284
         dtype: float64
In [33]: | 1 # which columns were kept?
         2 wine feature names[logr l1.coef [0] != 0]
Out[33]: array(['alcohol', 'proline'], dtype=object)
```

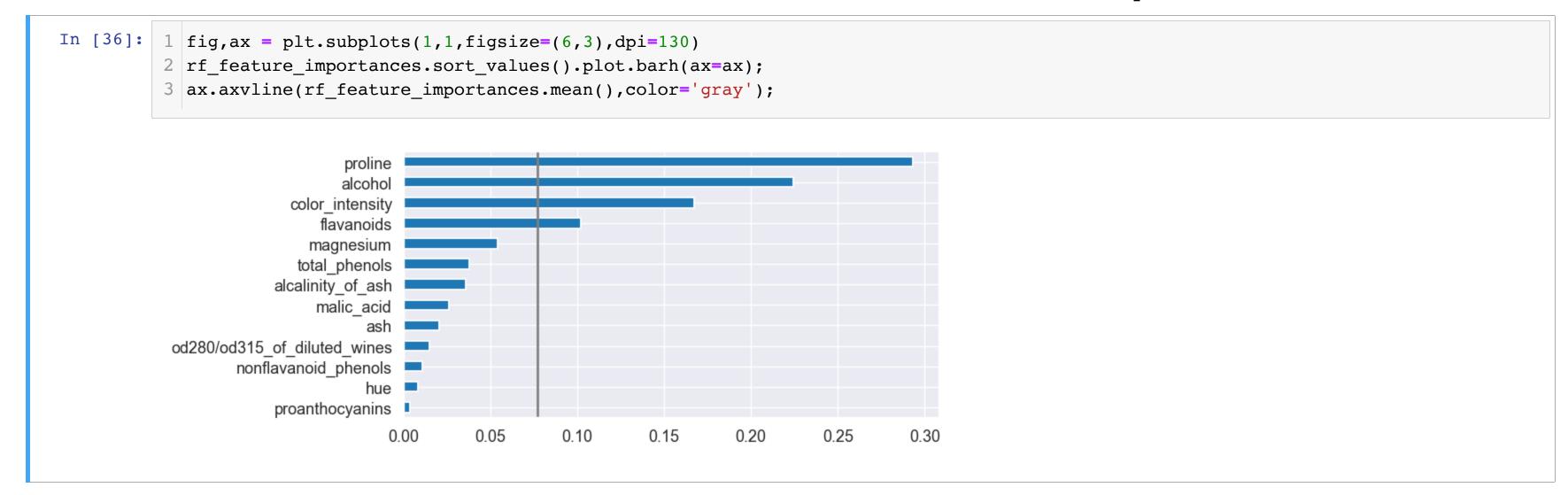
- Trees choose questions based on removing impurity
- We can rank the feature based on how much impurity they remove

- 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]: 1 from sklearn.ensemble import RandomForestClassifier
         3 rf = RandomForestClassifier(random state=0).fit(X train zscore, y train)
         4 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, 0.2931)
In [35]: 1 rf feature importances = pd.Series(rf.feature importances ,index=wine feature names)
         2 rf feature importances.sort values(ascending=False).round(3)
Out[35]: proline
                                          0.293
         alcohol
                                         0.225
         color intensity
                                         0.167
         flavanoids
                                         0.102
         magnesium
                                         0.054
         total phenols
                                         0.038
         alcalinity of ash
                                         0.036
         malic acid
                                         0.026
         ash
                                         0.021
         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]: 1 from sklearn.feature selection import SelectFromModel
         3 sfm lr = SelectFromModel(logr 11,
                                    threshold=None, # if model uses 11 regularization: abs val > 1e-5, otherwise mean
                                                    # don't need to refit, but may give warnings about missing feature manes
                                    prefit=True,
          6
         8 sfm lr.get support() # boolean mask of features selected
Out[37]: array([ True, False, False, False, False, False, False, False, False,
                False, False, True])
In [38]: 1 wine feature names[sfm lr.get support()]
Out[38]: array(['alcohol', 'proline'], dtype=object)
In [39]: 1 X train subset = sfm lr.transform(X train zscore)
         2 X train subset.shape
         /Users/andi/miniconda3/envs/sigma2/lib/python3.8/site-packages/sklearn/base.py:443: UserWarning: X has feature names, but Selec
         tFromModel was fitted without feature names
           warnings.warn(
Out[39]: (97, 2)
```

```
In [37]: 1 from sklearn.feature selection import SelectFromModel
         3 sfm lr = SelectFromModel(logr 11,
                                    threshold=None, # if model uses 11 regularization: abs val > 1e-5, otherwise mean
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                                    prefit=True,
          6
         8 sfm lr.get support() # boolean mask of features selected
Out[37]: array([ True, False, False, False, False, False, False, False, False,
                False, False, False, True])
In [38]: 1 wine feature names[sfm lr.get support()]
Out[38]: array(['alcohol', 'proline'], dtype=object)
In [39]: 1 X_train_subset = sfm_lr.transform(X_train_zscore)
         2 X train subset.shape
         /Users/andi/miniconda3/envs/sigma2/lib/python3.8/site-packages/sklearn/base.py:443: UserWarning: X has feature names, but Selec
         tFromModel was fitted without feature names
           warnings.warn(
Out[39]: (97, 2)
In [40]: 1 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]]
```

### Feature Selection: SelectFromModel Cont.

### Feature Selection: SelectFromModel Cont.

### Feature Selection: SelectFromModel Cont.

```
In [41]: 1 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)
         6 wine feature names[sfm rf.get support()]
Out[41]: array(['alcohol', 'magnesium', 'color_intensity', 'proline'], dtype=object)
In [42]: 1 sfm_rf.estimator_.feature_importances_.mean().round(3)
Out[42]: 0.077
In [43]: 1 sfm_rf_feature_importances = pd.Series(sfm_rf.estimator_.feature_importances_,index=wine_feature_names)
         2 sfm_rf_feature_importances.sort_values(ascending=False).round(3)
Out[43]: proline
                                         0.279
         alcohol
                                         0.254
         color intensity
                                         0.168
         magnesium
                                         0.079
         flavanoids
                                         0.059
         alcalinity of ash
                                         0.036
         total phenols
                                         0.035
         malic acid
                                         0.022
         od280/od315 of diluted wines
                                         0.020
                                         0.016
         ash
                                         0.013
         hue
         proanthocyanins
                                         0.010
         nonflavanoid phenols
                                         0.009
         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

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- Instead recursively select smaller subsets of features
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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  $\mathbb{R}^2$
- $\mathbb{R}^2$  describes the proportion of explained variance
- Additional features explain more 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

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

Is this due to a better model or just adding features?

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```
In [48]: 1 print('Adj R2 with 3 features :',adj_r2(lr.fit(X_r.iloc[:,:3],y_r),X_r.iloc[:,:3],y_r).round(2))
2 print('Adj R2 with all features :',adj_r2(lr.fit(X_r.iloc[:,:],y_r),X_r.iloc[:,:],y_r).round(2))
Adj R2 with 3 features : 0.35
Adj R2 with all features : 0.62
```

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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]: 1 from statsmodels.api import OLS
             3 \mod = OLS(y r, X r).fit()
            4 print(model.rsquared adj.round(3))
             5 model.summary()
            0.621
Out[49]:
           OLS Regression Results
                                               R-squared (uncentered):
             Dep. Variable:
                              alcohol
                                                                         0.668
                              OLS
                                               Adj. R-squared (uncentered): 0.621
             Model:
             Method:
                              Least Squares
                                               F-statistic:
                                                                         14.23
                              Wed, 11 Dec 2024 Prob (F-statistic):
                                                                         1.06e-15
             Date:
                              23:26:03
                                               Log-Likelihood:
                                                                         -84.207
             Time:
                                                                         192.4
             No. Observations: 97
                                               AIC:
             Df Residuals:
                              85
                                               BIC:
                                                                         223.3
                              12
             Df Model:
             Covariance Type: nonrobust
                                                                      [0.025 0.975]
                                                 std err t
                                         coef
             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
                                                        0.079
                                                                0.937
                                                                      -0.146 0.158
             magnesium
                                         0.0060 0.077
             total phenols
                                         0.0701
                                                 0.126
                                                        0.555
                                                                0.580
                                                                       -0.181 0.321
                                                                      -0.338 0.390
             flavanoids
                                         0.0260
                                                0.183
                                                        0.142
                                                                0.888
             nonflavanoid_phenols
                                         0.0545 0.086
                                                        0.631
                                                                0.530
                                                                      -0.117 0.226
                                                                      -0.304 0.022
             proanthocyanins
                                         -0.1407 0.082
                                                        -1.717
                                                               0.090
             color_intensity
                                         0.3190
                                                 0.138
                                                        2.316
                                                                0.023 0.045
                                                                             0.593
                                         0.1609 0.074 2.183
                                                               0.032 0.014 0.308
             hue
```

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

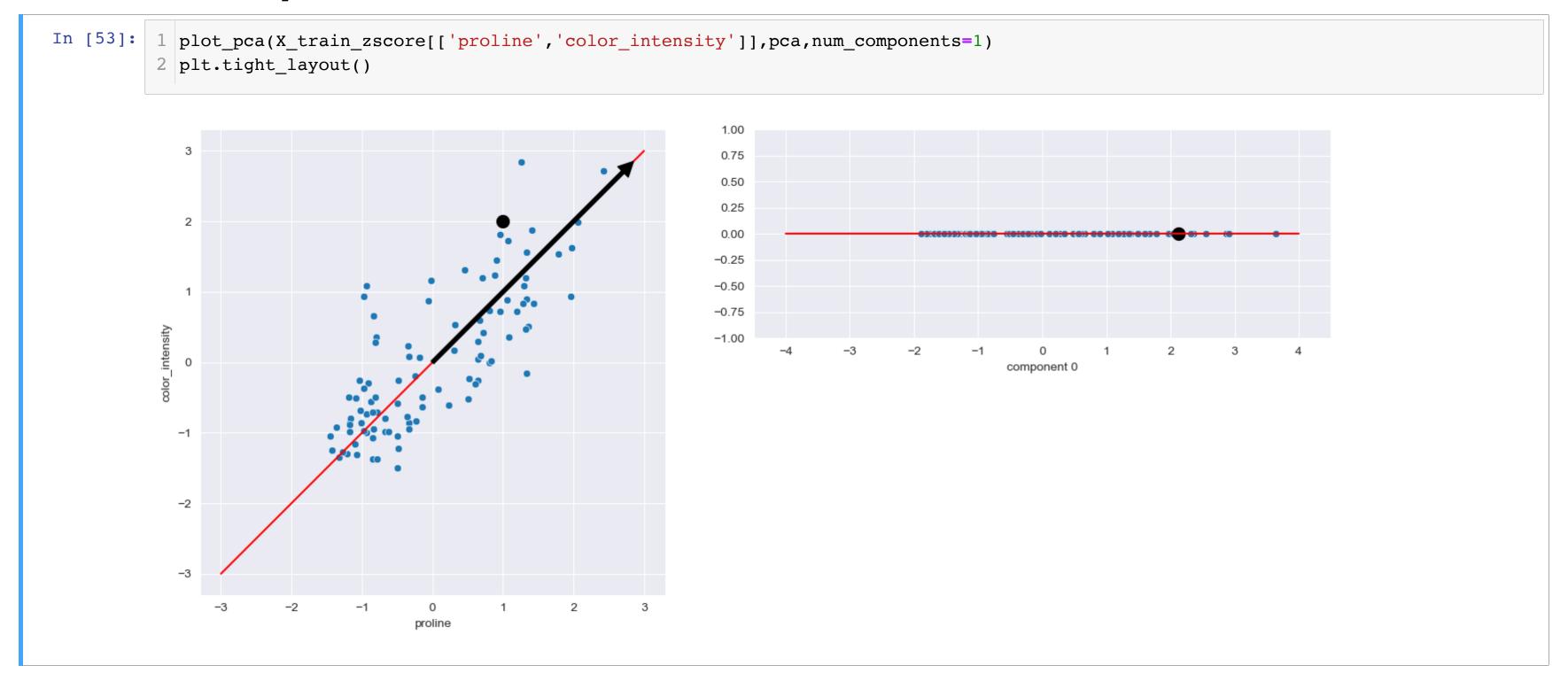
## Principal Component Analysis (PCA)

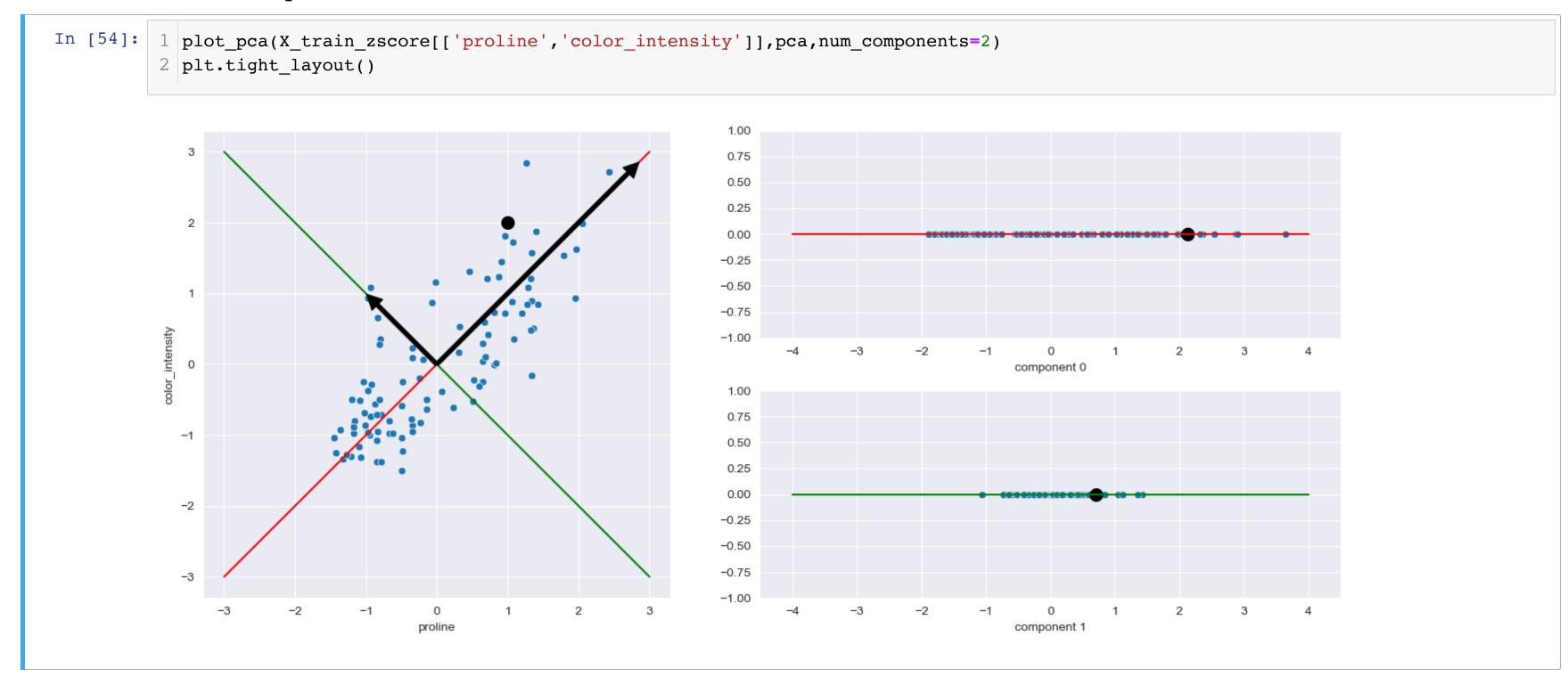
- How it works:
  - O. first center the data (subtract the means)
  - 1. extract first component:
    - direction (combination of features)
    - explains maximum variance
  - 2. extract next component:
    - direction, orthogonal to the first (linearly independent)
    - explains max remaining variance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

# **PCA Example**

## **PCA Example**

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





### PCA in sklearn

### PCA in sklearn

### PCA in sklearn

```
In [55]: 1 from sklearn.decomposition import PCA
         3 pca = PCA().fit(X_train_zscore)
         5 print(f'num input features: {X_train_zscore.shape[1]}')
         6 print(f'num pca components: {pca.n_components_}')
         num input features: 13
         num pca components: 13
In [56]: 1 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, 0.391)
In [57]: 1 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**

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

```
In [58]: 1 pca = PCA().fit(X_train_zscore)
        5 print(f'cumulative explained variance : {pca.explained_variance_ratio_.cumsum().round(2)}')
        6 df_var = pd.DataFrame({'component':range(pca.n_components_),
                               'cumulative explained variance':pca.explained_variance_ratio_.cumsum()})
        8 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
          0.8
          0.7
          0.4
```

## Dimensionality Reduction with PCA

### Dimensionality Reduction with PCA

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

### Example Dataset: Labeled Faces in th Wild (LFW)

#### Labeled Faces in the Wild

```
In [60]: 1 from sklearn.datasets import fetch_lfw_people
         3 lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.6)
In [61]: 1 [lfw_people.target_names[i] for i in range(6)]
Out[61]: ['Ariel Sharon',
          'Colin Powell',
          'Donald Rumsfeld',
          'George W Bush',
          'Gerhard Schroeder',
          'Hugo Chavez']
In [62]: 1 sns.set_style('dark')
         2 plt.imshow(lfw_people.images[1], cmap=plt.cm.gray, vmin=0, vmax=1)
         3 plt.title(lfw_people.target_names[lfw_people.target[1]], size=12);
                    Tony Blair
          20
          30
```

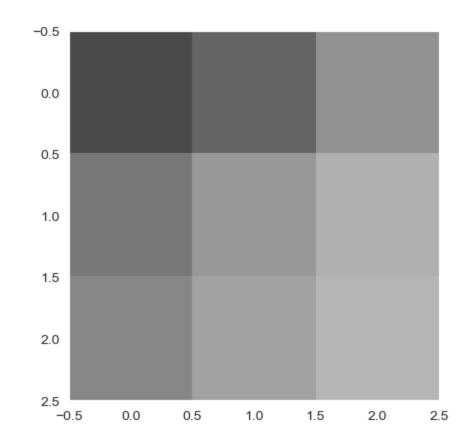
# **Example Pixel Values**

# **Example Pixel Values**

```
In [63]: 1 # sample of 3x3 set of pixels
          2 plt.imshow(lfw_people.images[1][20:23,20:23],cmap=plt.cm.gray,vmin=0, vmax=1);
           -0.5
           0.0
           0.5
           1.0
           1.5
           2.0
                       0.5
                            1.0
                                 1.5
```

### **Example Pixel Values**

```
In [63]: 1 # sample of 3x3 set of pixels
2 plt.imshow(lfw_people.images[1][20:23,20:23],cmap=plt.cm.gray,vmin=0, vmax=1);
```



```
In [65]: 1 lfw_people.images[1].shape
Out[65]: (75, 56)
```

```
In [65]: 1 lfw_people.images[1].shape
Out[65]: (75, 56)
In [66]: 1 x = lfw_people.images[1].reshape(1,-1)
2 x
Out[66]: array([[0.00261438, 0.00261438, 0. , ..., 0.01830065, 0. , ..., 0.1830065, 0. , ..., 0.1830065, 0. )
```

• Grid as a fixed length feature vector?

What information do we lose when we do this?

#### Create a Dataset

#### Create a Dataset

```
In [68]: | 1 # get the shape of images for plotting the
          2 n_samples, h, w = lfw_people.images.shape
          4 # use actual pixel values, ignoring relative position
          5 X faces = lfw people.data
          6 n_features = X_faces.shape[1]
         8 # the label to predict is the id of the person
         9 y faces = lfw people.target
        10 target names = lfw people.target names
        11 n_classes = target_names.shape[0]
        12
        13 # create train/test split
        14 X_train_faces, X_test_faces, y_train_faces, y_test_faces = train_test_split(X_faces, y_faces,
        15
                                                                                       test size=0.25,
        16
                                                                                       stratify=y faces,
        17
                                                                                       random state=0)
        18 print(f"image size: {h}x{w}")
        19 print("n_features: %d" % n_features)
        20 print("n_classes : %d" % n_classes)
         21 print(f"n_train : {len(X_train_faces)}")
         22 print(f"n test
                             : {len(X test faces)}")
         image size: 75x56
         n features: 4200
         n classes : 7
         n train : 966
                 : 322
         n test
```

# Variance explained by PCA

### Variance explained by PCA

cumulative explained v 0.0 2.0 2.0

0.4

0.3

200

component

```
In [70]: | 1 # set the number of dimensions we want to retain
         2 n components = 200
         4 # instantiate and fit on X train
         5 pca faces = PCA(n components=n components,
                          svd solver='randomized',
                          whiten=True).fit(X_train_faces)
         9 # extract and reshape components into eigenfaces for plotting
        10 eigenfaces = pca_faces.components_.reshape((n_components, h, w))
        11
        12 # transform the training and test set for classification
        13 X train faces pca = pca faces.transform(X train faces)
        14 X test faces pca = pca faces.transform(X test faces)
In [71]: 1 pca faces.components [0].round(2)
Out[71]: array([0.01, 0.01, 0.01, ..., 0. , 0. ], dtype=float32)
In [72]: 1 pca faces.singular values .round(2)
Out[72]: 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 ,
                37.74, 35.97, 35.33, 34.61, 33.79, 32.88, 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, 15.84, 15.68, 15.67, 15.52, 15.45, 15.28, 15.13,
```

```
In [73]: 1 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(())
         10
                    plt.yticks(())
        11
                plt.tight layout()
        12
        13 # plot the result of the prediction on a portion of the test set
        14 def title(y pred, y test, target names, i):
                pred_name = target_names[y_pred[i]].rsplit(' ', 1)[-1]
         15
                true_name = target_names[y_test[i]].rsplit(' ', 1)[-1]
        16
                return 'predicted: %s\ntrue: %s' % (pred_name, true_name)
        17
```



### **Train and Tune SVC**

#### **Train and Tune SVC**

#### **Train and Tune SVC**

#### **Evaluate on the test set**

#### **Evaluate on the test set**

```
In [77]: 1 from sklearn.metrics import classification_report
         3 y_pred_pca = clf_faces_pca.predict(X_test_faces_pca)
         4 print(classification_report(y_test_faces, y_pred_pca, target_names=target_names))
                            precision
                                         recall f1-score
                                                            support
              Ariel Sharon
                                 0.52
                                           0.58
                                                     0.55
                                                                 19
              Colin Powell
                                 0.73
                                           0.76
                                                     0.74
                                 0.74
                                           0.67
                                                     0.70
           Donald Rumsfeld
                                                                 30
                                           0.89
             George W Bush
                                 0.80
                                                     0.85
                                                                133
         Gerhard Schroeder
                                 0.65
                                           0.41
                                                     0.50
                                                                 27
                                 0.89
                                           0.44
                                                     0.59
               Hugo Chavez
                                                                 18
                                           0.78
                Tony Blair
                                 0.74
                                                     0.76
                                                                 36
                                                     0.75
                                                                322
                  accuracy
                                                     0.67
                                                                322
                 macro avg
                                 0.72
                                           0.65
              weighted avg
                                 0.75
                                           0.75
                                                     0.74
                                                                322
```

# **Prediction Examples**

#### **Prediction Examples**



#### Performance without PCA: Train

#### Performance without PCA: Train

```
1 %%time
3 # Warning: this cell takes up to 3 minutes to execute on an Intel i7 1.8Ghz w/ 8 cores
5 params = {'C': [1e3, 5e3, 1e4, 5e4, 1e5],
            'gamma': [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.1],}
7 clf faces nopca = GridSearchCV(SVC(kernel='rbf', class weight='balanced'),
                                     params, cv=3, n jobs=-1)
9 clf faces nopca = clf faces nopca.fit(X train faces, y train faces)
10
1 #CPU times: user 2.08 s, sys: 53.3 ms, total: 2.13 s
12#Wall time: 2min 42s
13
14print(f"best params : {clf faces nopca.best params }")
15print(f"best score : {clf faces nopca.best score :0.2f}")
16
1 #best_params : {'C': 1000.0, 'gamma': 0.0001}
18#best score : 0.78
```

#### Performance without PCA: Evaluate

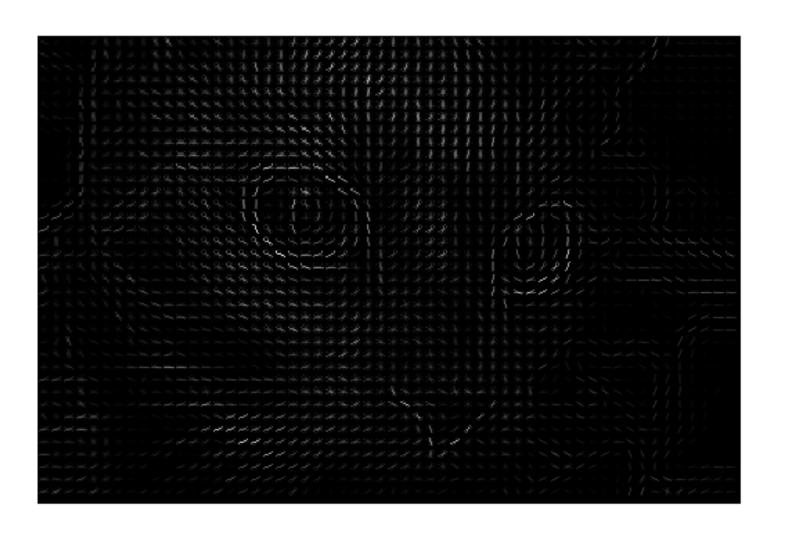
#### Performance without PCA: Evaluate

```
1 y pred_nopca = clf_faces_nopca.predict(X_test_faces)
2 print(classification_report(y_test_faces, y_pred_nopca, target_names=target_names))
3
4 #
                      precision
                                  recall f1-score
                                                     support
5
6 #
        Ariel Sharon
                           0.65
                                     0.79
                                              0.71
                                                          19
        Colin Powell
                           0.82
                                     0.69
                                              0.75
                                                          59
                                              0.60
8 #
     Donald Rumsfeld
                          0.60
                                    0.60
                                                          30
9 #
                                    0.90 0.86
                          0.82
                                                         133
       George W Bush
                          0.56
                                    0.56 0.56
                                                          27
   Gerhard Schroeder
1 1#
                                    0.28 0.40
         Hugo Chavez
                          0.71
                                                          18
12#
          Tony Blair
                           0.71
                                     0.75
                                              0.73
                                                          36
13
14#
                                              0.75
                                                         322
            accuracy
15#
                           0.70
                                              0.66
                                                         322
           macro avq
                                     0.65
16#
        weighted avg
                                              0.74
                                                         322
                           0.75
                                     0.75
```

### Other Image Recognition Methods

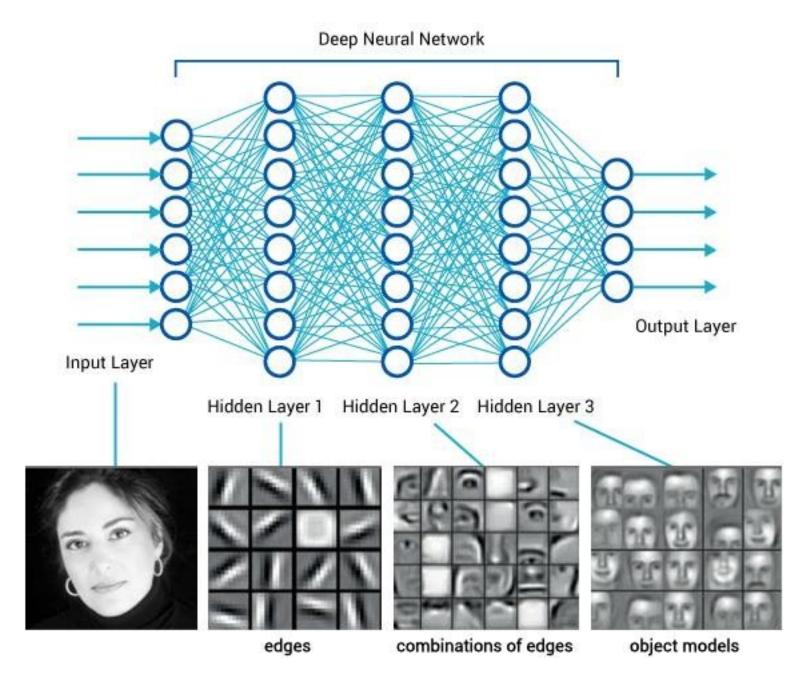
- With Feature Engineering and general models
  - ex: Histogram of Oriented Gradients or HOG (See PDSH Chap 5)
  - many more (See <u>scikit-image</u>)





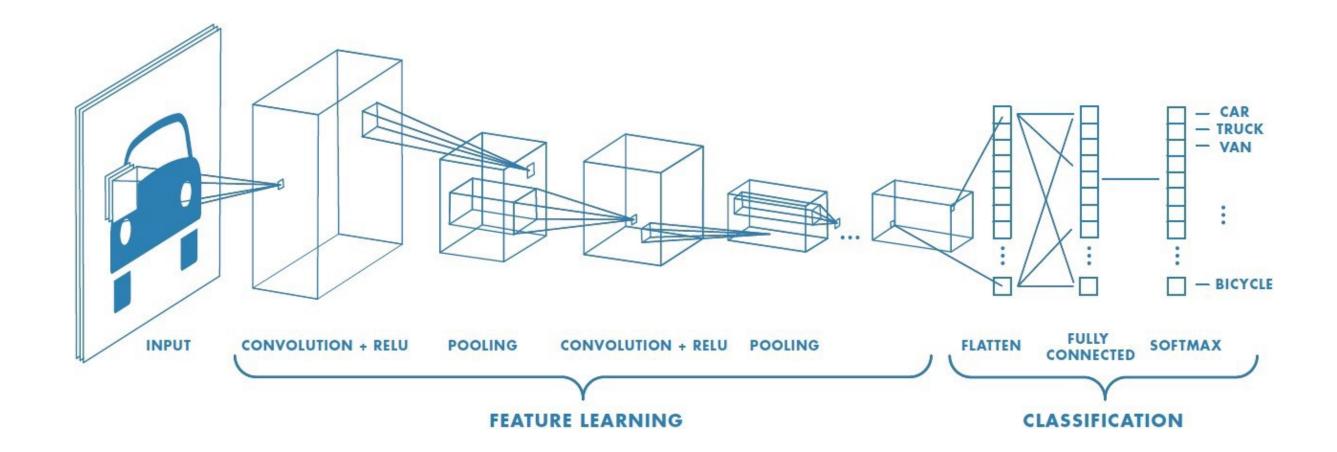
### Other Image Recognition Methods: Deep Neural Networks

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