

Elements Of Data Science - F2021

Week 9: Dimensionality Reduction, Feature Selection and Feature Extraction

11/15/2021

TODOs

- Readings:
 - PML Chapter 6, first 3 sections on Pipelines
 - PML Chapter 8: Applying Machine Learning to Sentiment Analysis
- Quiz 9, Due **Sunday Nov 21st, 11:59pm ET**
- HW3, Due **Tues Nov 23 at 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^2**
 - **Feature Extraction**
 - PCA
- **Example: Image Recognition Using PCA**
- **Pipelines?**

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
```

Joining Datasets

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

Joining 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'])
```


Joining 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
0	1001	iris
1	1002	rose

	flower_id	price
0	1002	3.99
1	1003	2.25

Joining Datasets On Index

- easiest way to join in Pandas 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
0	1001	iris
1	1002	rose

Joining Datasets On Index

- easiest way to join in Pandas 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
0	1001	iris
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

Joining Datasets On Index

- easiest way to join in Pandas 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
0	1001	iris
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.copy()
df_flower_price.set_index('flower_id',inplace=True)
df_flower_price
```

Out[7]:

	price
flower_id	
1002	3.99
1003	2.25

Joining Datasets in Pandas On Index Using `df.join()`

Joining Datasets in Pandas On Index Using `df.join()`

```
In [8]: display(df_flower_name)
display(df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

Joining Datasets in Pandas On Index Using `df.join()`

```
In [8]: display(df_flower_name)
display(df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

```
In [9]: df_flower_name.join(df_flower_price)
```

Out[9]:

name price		
flower_id		
1001	iris	NaN
1002	rose	3.99

Joining Datasets in Pandas On Index Using `df.join()`

```
In [8]: display(df_flower_name)
display(df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

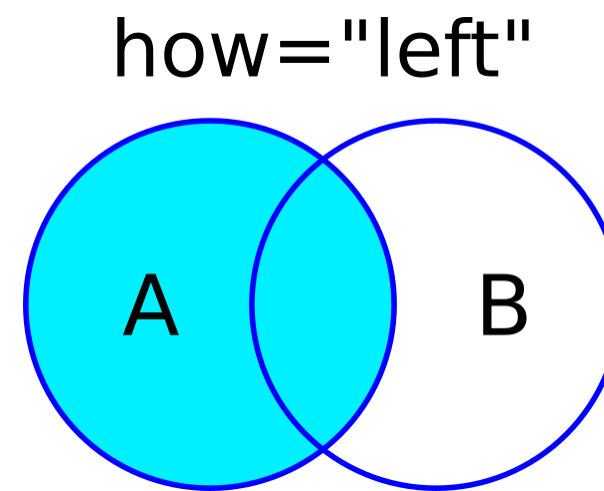
```
In [9]: df_flower_name.join(df_flower_price)
```

Out[9]:

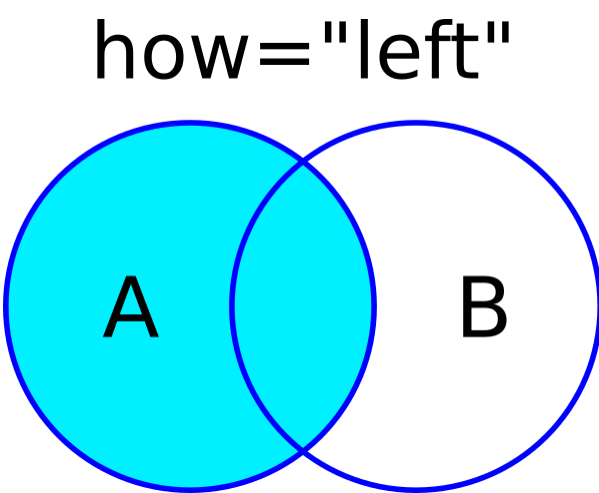
	name	price
flower_id		
1001	iris	NaN
1002	rose	3.99

- by default, this is a 'Left Join'

Join Types: Left Join



Join Types: Left Join

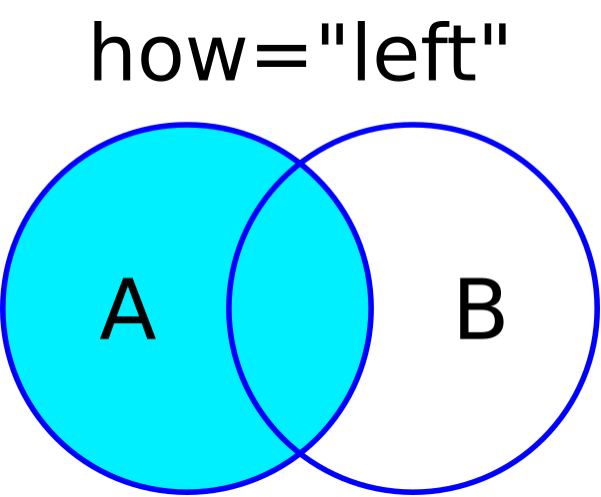


```
In [10]: display(df_flower_name,df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

Join Types: Left Join



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

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

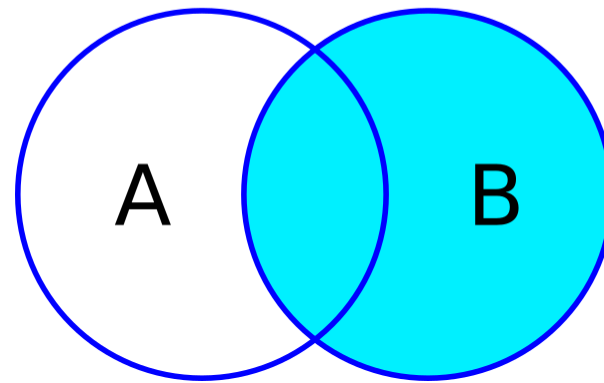
```
In [11]: df_flower_name.join(df_flower_price,how="left") # default for df.join() is left join
```

Out[11]:

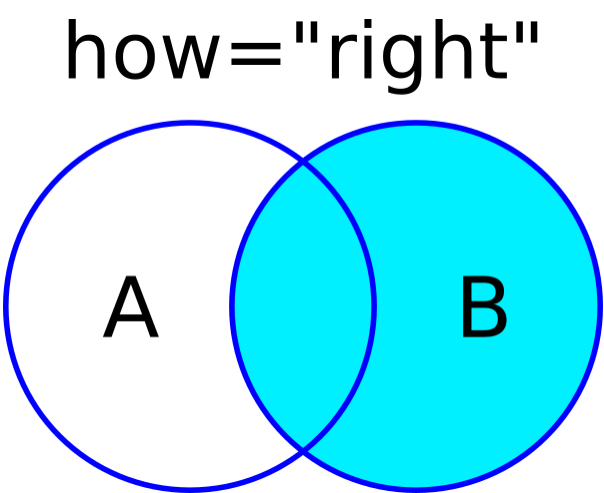
name price		
flower_id		
1001	iris	NaN
1002	rose	3.99

Join Types: Right Join

how="right"



Join Types: Right Join

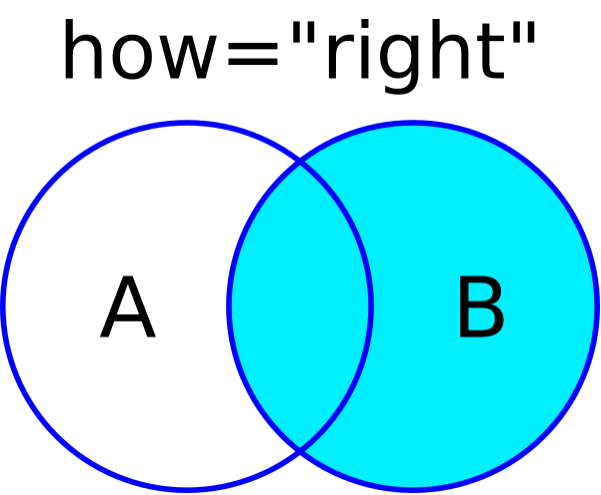


```
In [12]: display(df_flower_name,df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

Join Types: Right Join



```
In [12]: display(df_flower_name,df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

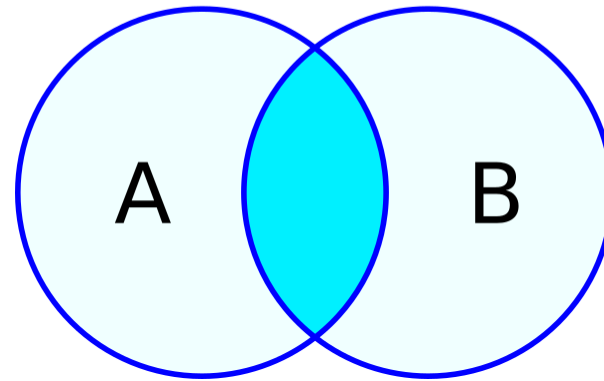
```
In [13]: df_flower_name.join(df_flower_price,how='right')
```

Out[13]:

name price		
flower_id		
1002	rose	3.99
1003	NaN	2.25

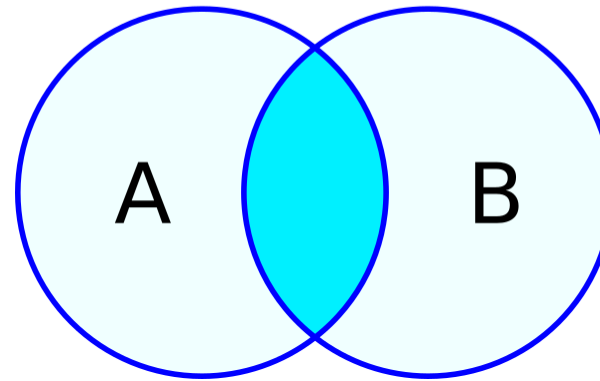
Join Types: Inner Join

how="inner"



Join Types: Inner Join

how="inner"

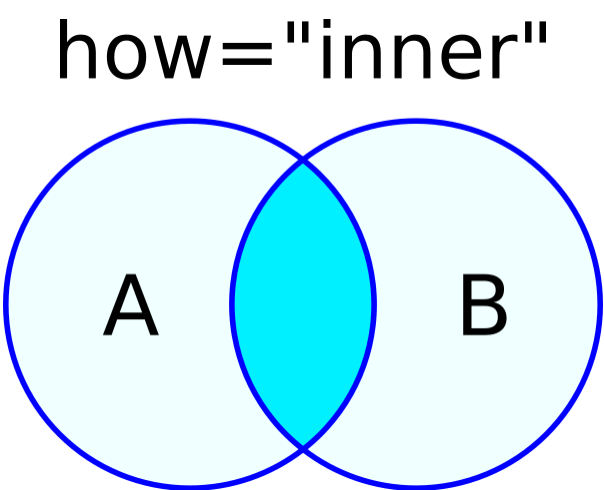


```
In [14]: display(df_flower_name,df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

Join Types: Inner Join



```
In [14]: display(df_flower_name,df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

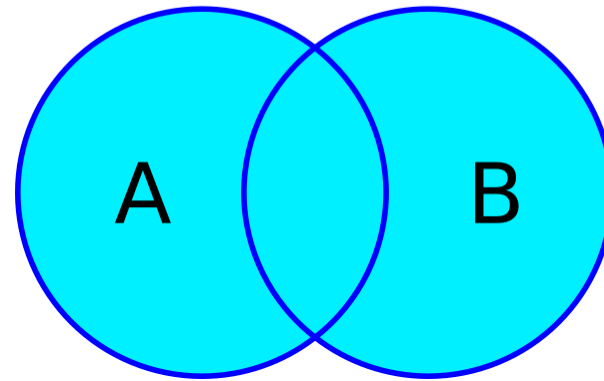
```
In [15]: df_flower_name.join(df_flower_price,how='inner')
```

Out[15]:

name price		
flower_id		
1002	rose	3.99

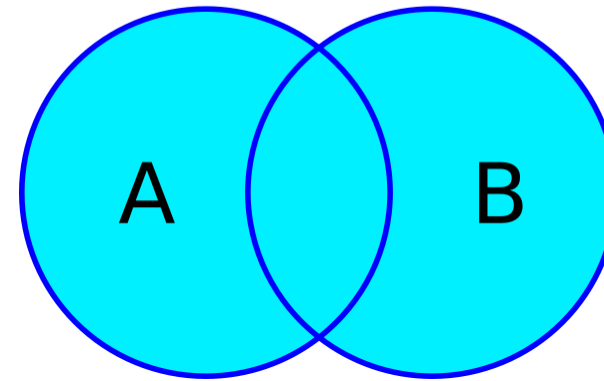
Join Types: Outer Join

how="outer"



Join Types: Outer Join

how="outer"



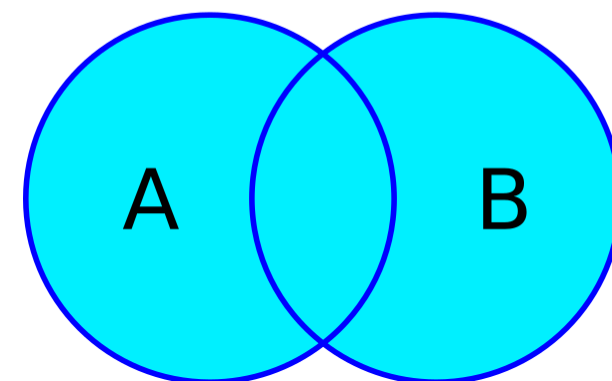
```
In [16]: display(df_flower_name, df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	3.99
1003	2.25

Join Types: Outer Join

how="outer"



```
In [16]: display(df_flower_name,df_flower_price)
```

name	
flower_id	
1001	iris
1002	rose

price	
flower_id	
1002	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=`

Setting the Index When Reading in Data

- instead of using `.set_index()`, can specify `index_col=`

```
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=`

```
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

```
In [19]: # can set the index when reading in the csv
pd.read_csv('../data/flowershop_data_with_dups.csv',
            index_col='purchase_id')
        ).head(2)
```

Out[19]:

	lastname	purchase_date	stars	price	favorite_flower
purchase_id					
1000	PERKINS	2017-04-08	5	19.599886	iris
1001	ROBINSON	2017-01-01	5	37.983904	NaN

Joining on the Index using `.join()`

Joining on the Index using `.join()`

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

Out[20]:

name	
flower_id	
1001	iris
1002	rose

Joining on the Index using `.join()`

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

Out[20]:

name	
flower_id	
1001	iris
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	1	0
1002	0	1

Joining on the Index using `.join()`

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

Out[20]:

name	
flower_id	
1001	iris
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	1	0
1002	0	1

```
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	0
1002	rose	0	1

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,
         df_flower_price,
         left_on='flower_id',
         right_on='flower_id') # what is the default join for merge?
```

Out[23]:

	name	price
flower_id		
1002	rose	3.99

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,
         df_flower_price,
         left_on='flower_id',
         right_on='flower_id') # what is the default join for merge?
```

Out[23]:

	name	price
flower_id		
1002	rose	3.99

```
In [24]: # if both id columns have the same name, use on
pd.merge(df_flower_name,
         df_flower_price,
         on='flower_id',
         how='outer')
```

Out[24]:

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

Joining Datasets Review

- Use `.join()` when you can, using dataframe indices
- May need to set the dataframe indices (`.set_index()` or `index_col=`)
- Know the different general join types: Left, Right, Inner, Outer
- Use `pd.merge()` when you need something more complicated

Questions?

Dimensionality Reduction

Recall: Methods for Avoiding Overfitting

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

Dimensionality Reduction

- Reasons to reduce the number of features:
 - improve *model performance* (reducing complexity reducing chance of overfitting)
 - improve *speed performance* (reducing 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 import datasets
from sklearn.model_selection import train_test_split

wine = datasets.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]
y_wine = y_wine[y_wine < 2]

X_train, X_test, y_train, y_test = train_test_split(X_wine, y_wine, random_state=0)
X_train.columns.values
```

```
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

```
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X_wine = pd.DataFrame(wine.data, columns=wine.feature_names)
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# reduce to binary classification
X_wine = X_wine.iloc[y_wine < 2]
y_wine = y_wine[y_wine < 2]

X_train, X_test, y_train, y_test = train_test_split(X_wine, y_wine, random_state=0)
X_train.columns.values
```

```
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	proline
76	13.03	0.90	1.71	16.0	86.0	1.95	2.03	0.24	1.46	4.60	1.19	2.48	392.0
78	12.33	0.99	1.95	14.8	136.0	1.90	1.85	0.35	2.76	3.40	1.06	2.31	750.0
45	14.21	4.04	2.44	18.9	111.0	2.85	2.65	0.30	1.25	5.24	0.87	3.33	1080.0

Need to Standardize Features

```
In [27]: X_train.agg(['mean', 'std']).T.sort_values('mean', ascending=False)
```

Out[27]:

	mean	std
proline	770.381443	351.632012
magnesium	99.649485	15.215837
alcalinity_of_ash	18.926804	3.162986
alcohol	12.876392	0.882710
color_intensity	4.112680	1.660242
od280/od315_of_diluted_wines	2.933299	0.452246
total_phenols	2.479175	0.537158
flavanoids	2.426598	0.672639
ash	2.338660	0.279052
malic_acid	2.033402	0.979120
proanthocyanins	1.732474	0.520371
hue	1.054082	0.179279
nonflavanoid_phenols	0.329794	0.105574

Standardize Features

Standardize Features

```
In [28]: from sklearn.preprocessing import StandardScaler  
  
ss = StandardScaler()  
X_train = pd.DataFrame(ss.fit_transform(X_train), columns=X_train.columns)  
  
X_test = ss.transform(X_test)
```

Standardize Features

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

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

X_test = ss.transform(X_test)
```

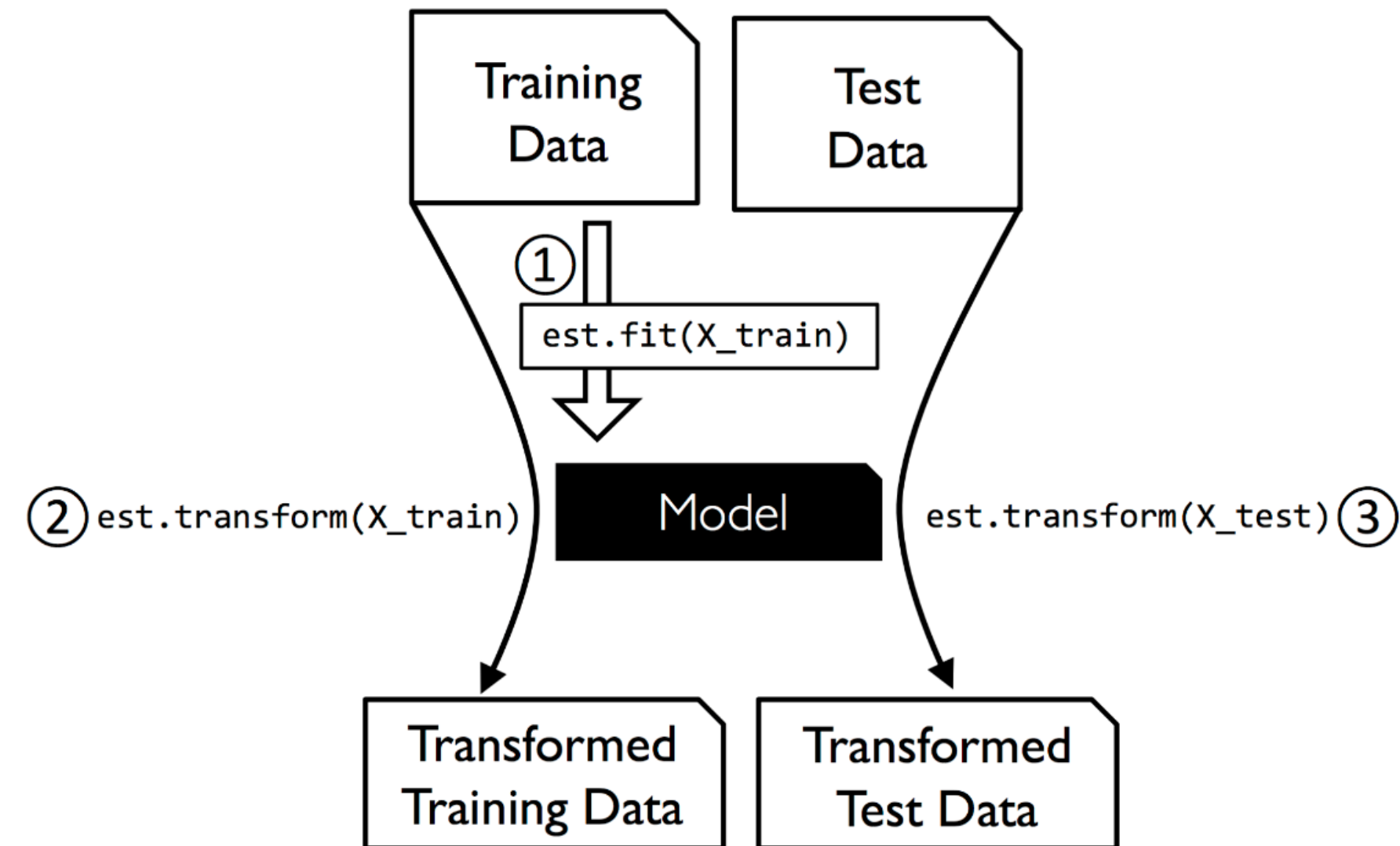
```
In [29]: X_train.agg(['mean', 'std']).T.sort_values('mean', ascending=False)
```

Out[29]:

	mean	std
total_phenols	2.028160e-15	1.005195
flavanoids	6.638447e-16	1.005195
alcalinity_of_ash	4.727032e-16	1.005195
magnesium	3.694067e-16	1.005195
alcohol	1.281907e-16	1.005195
proline	-3.204767e-17	1.005195
proanthocyanins	-1.110223e-16	1.005195
nonflavanoid_phenols	-2.495140e-16	1.005195
color_intensity	-4.051742e-16	1.005195
malic_acid	-4.229149e-16	1.005195
od280/od315_of_diluted_wines	-9.694422e-16	1.005195
hue	-1.818706e-15	1.005195
ash	-2.128881e-15	1.005195

Recall: Predicting vs Transforming with Train/Test Split

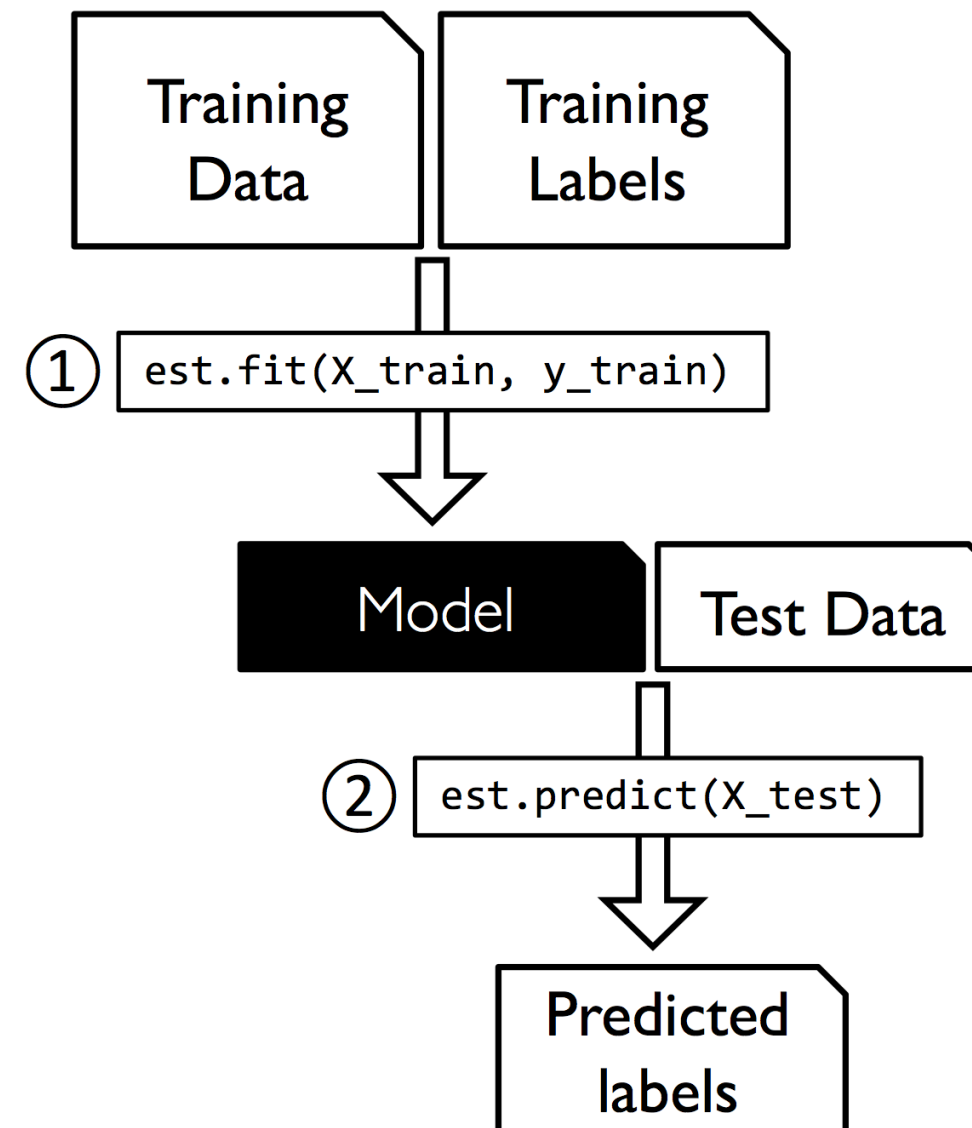
- When transforming data, fit on the training set, transform both train and test



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 the 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 **l1** regularization drives the coefficient of uninformative features to 0

Feature Selection: LASSO (L1)

- LASSO or ℓ_1 or `l1` 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(C=100, penalty="l1", solver="liblinear", random_state=123)
logr.fit(X_train, y_train)
logr.coef_[0,:5]
```

```
Out[30]: array([-5.74709641, -1.20824931, -2.70057811,  2.47398434, -0.28304842])
```


Feature Selection: LASSO (L1)

- LASSO or ℓ_1 or `l1` 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(C=100, penalty="l1", solver="liblinear", random_state=123)
logr.fit(X_train, y_train)
logr.coef_[0,:5]
```

```
Out[30]: array([-5.74709641, -1.20824931, -2.70057811,  2.47398434, -0.28304842])
```

```
In [31]: sorted_tuples = sorted(list(zip(X_train.columns.values,logr.coef_[0])),key=lambda x:x[1],reverse=True)
for feature,coef in sorted_tuples:
    print(f'{feature:30s} : {coef: 0.3f}')
```

```
alcalinity_of_ash           :  2.474
proanthocyanins             :  1.144
hue                         :  1.069
nonflavanoid_phenols        :  0.000
total_phenols               : -0.146
magnesium                   : -0.283
flavanoids                  : -0.376
color_intensity             : -0.638
od280/od315_of_diluted_wines : -0.860
malic_acid                  : -1.208
ash                         : -2.701
alcohol                     : -5.747
proline                     : -7.568
```

Feature Selection: LASSO (L1) Cont.

Feature Selection: LASSO (L1) Cont.

```
In [32]: # Now with LASSO
logr = LogisticRegression(C=0.1, penalty="l1", solver="liblinear", random_state=123)
logr.fit(X_train, y_train)

sorted_tuples = sorted(list(zip(X_train.columns.values, logr.coef_[0])), key=lambda x: x[1], reverse=True)
for feature, coef in sorted_tuples:
    print(f'{feature:30s} : {coef: 0.3f}')
```

```
malic_acid           : 0.000
ash                  : 0.000
alcalinity_of_ash    : 0.000
magnesium            : 0.000
total_phenols        : 0.000
nonflavanoid_phenols : 0.000
proanthocyanins      : 0.000
color_intensity      : 0.000
hue                  : 0.000
od280/od315_of_diluted_wines : 0.000
flavanoids           : -0.007
alcohol              : -0.982
proline              : -1.102
```

Feature Selection: LASSO (L1) Cont.

```
In [32]: # Now with LASSO
logr = LogisticRegression(C=0.1, penalty="l1", solver="liblinear", random_state=123)
logr.fit(X_train, y_train)

sorted_tuples = sorted(list(zip(X_train.columns.values, logr.coef_[0])), key=lambda x: x[1], reverse=True)
for feature, coef in sorted_tuples:
    print(f'{feature:30s} : {coef: 0.3f}')
```

```
malic_acid           : 0.000
ash                  : 0.000
alcalinity_of_ash    : 0.000
magnesium            : 0.000
total_phenols        : 0.000
nonflavanoid_phenols : 0.000
proanthocyanins      : 0.000
color_intensity      : 0.000
hue                  : 0.000
od280/od315_of_diluted_wines : 0.000
flavanoids           : -0.007
alcohol              : -0.982
proline              : -1.102
```

```
In [33]: # which columns were kept?
X_train.columns[X_train.coef_[0] != 0]
```

```
Out[33]: Index(['alcohol', 'flavanoids', 'proline'], dtype='object')
```

Feature Selection: Tree Based Model Feature Importance

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

Feature Selection: Tree Based Model Feature Importance

- 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=123).fit(X_train,y_train)
rf.feature_importances_ # (normalized) total reduction of function measuring impurity
```

```
Out[34]: array([0.27332426, 0.01783127, 0.01145411, 0.05480187, 0.05158374,
                0.05521824, 0.10260545, 0.01117794, 0.01033494, 0.13339066,
                0.00759636, 0.0216486 , 0.24903258])
```

Feature Selection: Tree Based Model Feature Importance

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- We can rank the feature based on how much impurity they remove

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```

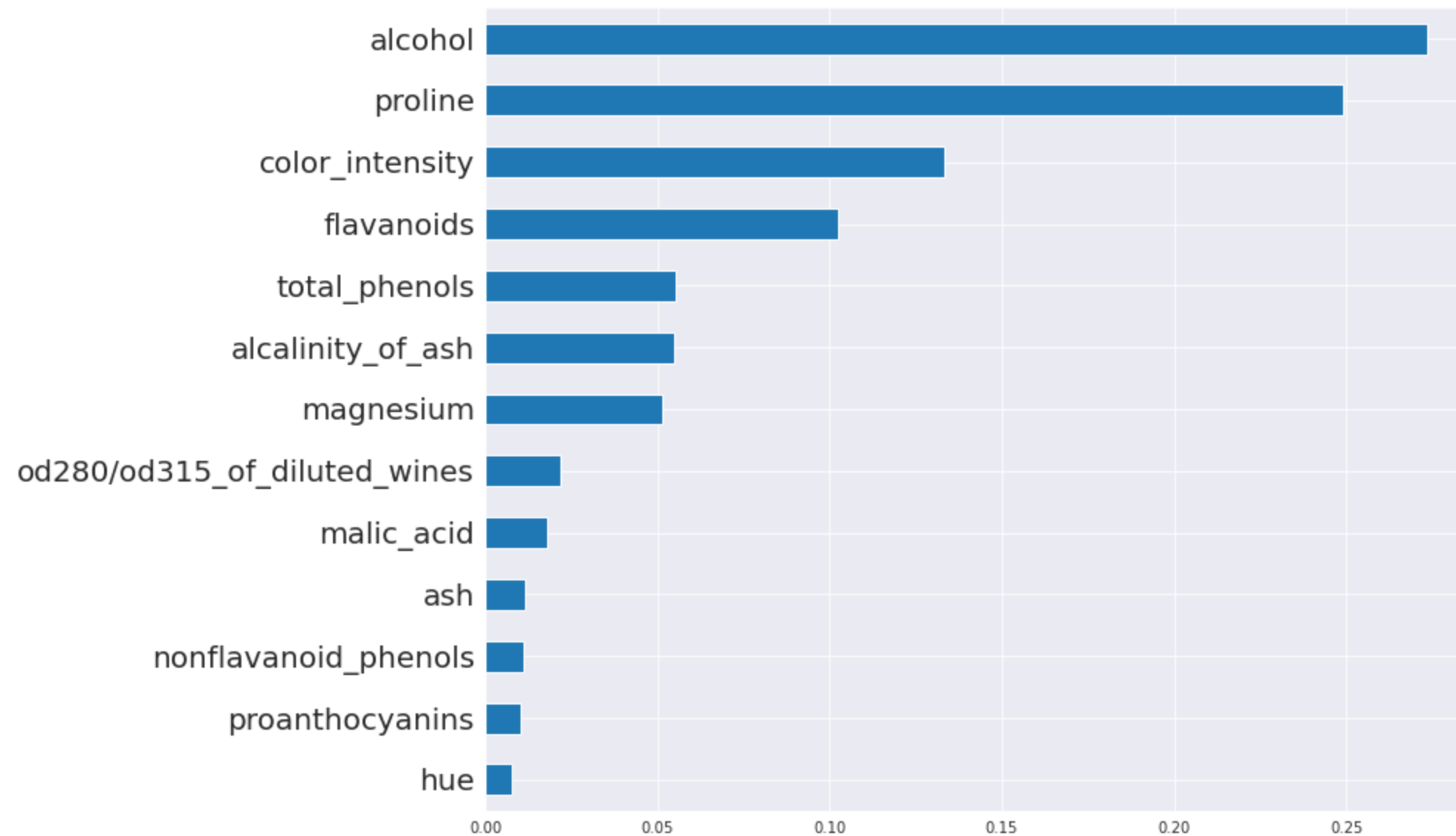
```
In [35]: feature_importances = pd.Series(rf.feature_importances_,index=X_train.columns)
feature_importances.sort_values(ascending=False).round(3)
```

```
Out[35]: alcohol          0.273
proline                  0.249
color_intensity         0.133
flavanoids              0.103
total_phenols           0.055
alcalinity_of_ash       0.055
magnesium               0.052
od280/od315_of_diluted_wines 0.022
malic_acid              0.018
ash                     0.011
nonflavanoid_phenols    0.011
proanthocyanins         0.010
hue                     0.008
dtype: float64
```

Feature Selection: Tree Based Model Feature Importance

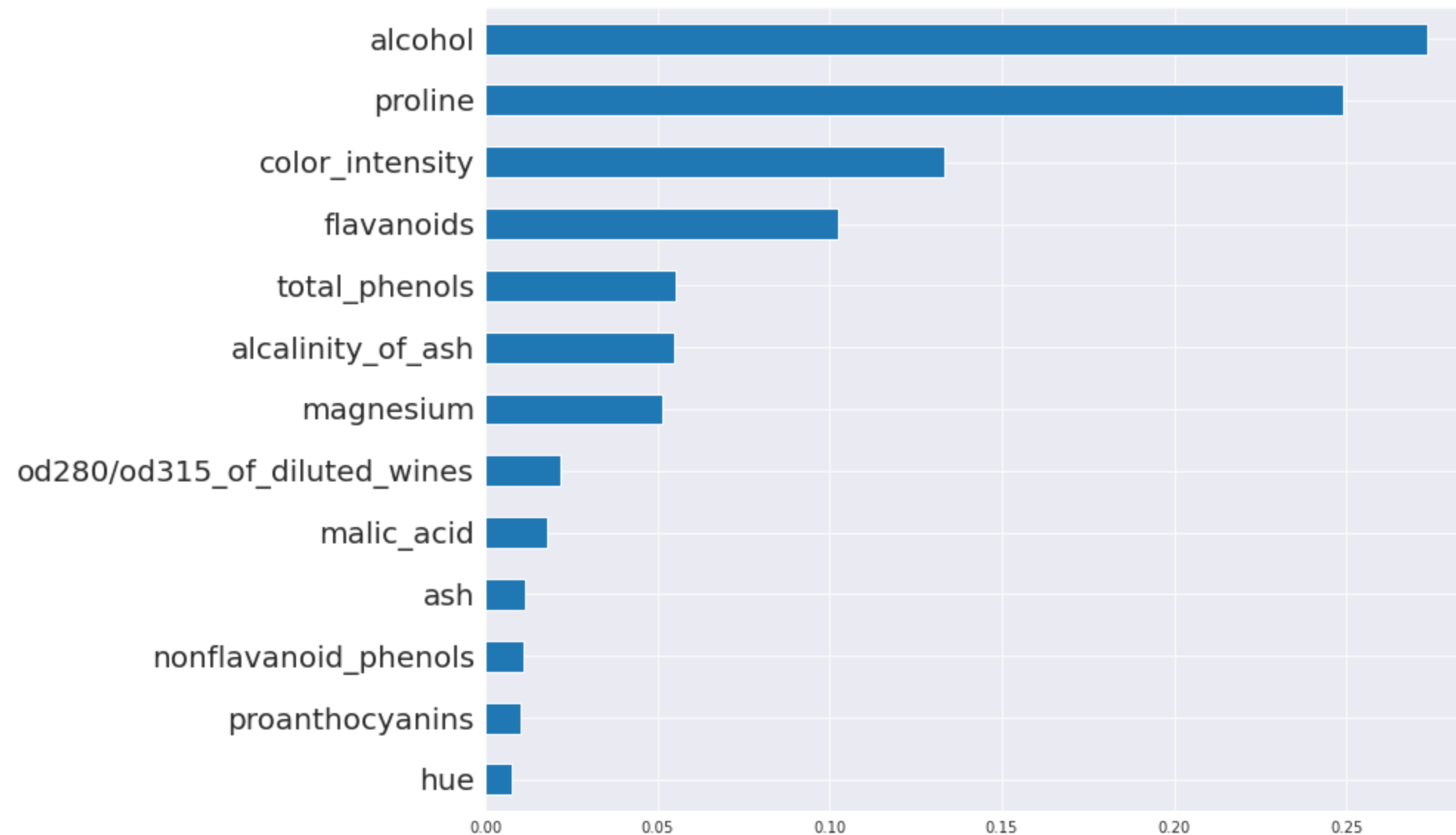
Feature Selection: Tree Based Model Feature Importance

```
In [36]: fig,ax = plt.subplots(1,1,figsize=(12,10))
feature_importances.sort_values().plot.barh(ax=ax);
ax.set_yticklabels(ax.get_yticklabels(),fontsize=20);
```



Feature Selection: Tree Based Model Feature Importance

```
In [36]: fig,ax = plt.subplots(1,1,figsize=(12,10))
feature_importances.sort_values().plot.barh(ax=ax);
ax.set_yticklabels(ax.get_yticklabels(),fontsize=20);
```



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

Feature Selection: SelectFromModel

Feature Selection: SelectFromModel

```
In [37]: from sklearn.feature_selection import SelectFromModel

sfm = SelectFromModel(logr,
                      threshold=None, # if model uses l1 regularization, anything greater than 1e-5, otherwise mean
                      prefit=True    # do not need to re-fit
                      )

sfm.get_support() # boolean mask of features selected
```

```
Out[37]: array([ True, False, False, False, False, False,  True, False, False,
                False, False, False,  True])
```

Feature Selection: SelectFromModel

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```
Out[37]: array([ True, False, False, False, False, False,  True, False, False,
                False, False, False,  True])
```

```
In [38]: x_train.columns[sfm.get_support()]
```

```
Out[38]: Index(['alcohol', 'flavanoids', 'proline'], dtype='object')
```

Feature Selection: SelectFromModel

```
In [37]: from sklearn.feature_selection import SelectFromModel
```

```
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                      )  
  
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```

```
Out[37]: array([ True, False, False, False, False, False,  True, False, False,  
                False, False, False,  True])
```

```
In [38]: X_train.columns[sfm.get_support()]
```

```
Out[38]: Index(['alcohol', 'flavanoids', 'proline'], dtype='object')
```

```
In [39]: X_train_subset = sfm.transform(X_train)  
X_train_subset.shape
```

```
Out[39]: (97, 3)
```

Feature Selection: SelectFromModel

```
In [37]: from sklearn.feature_selection import SelectFromModel
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```
sfm = SelectFromModel(logr,  
                      threshold=None, # if model uses l1 regularization, anything greater than 1e-5, otherwise mean  
                      prefit=True    # do not need to re-fit  
                      )  
  
sfm.get_support() # boolean mask of features selected
```

```
Out[37]: array([ True, False, False, False, False, False,  True, False, False,  
                False, False, False,  True])
```

```
In [38]: X_train.columns[sfm.get_support()]
```

```
Out[38]: Index(['alcohol', 'flavanoids', 'proline'], dtype='object')
```

```
In [39]: X_train_subset = sfm.transform(X_train)  
X_train_subset.shape
```

```
Out[39]: (97, 3)
```

```
In [40]: X_train_subset[:3] # note that this is no-longer a dataframe
```

```
Out[40]: array([[ 0.17492287, -0.59267761, -1.08166225],  
                [-0.62220886, -0.86167036, -0.05826353],  
                [ 1.51865922,  0.33385297,  0.88509284]])
```

Feature Selection: SelectFromModel Cont.

Feature Selection: SelectFromModel Cont.

```
In [41]: sfm_rf = SelectFromModel(RandomForestClassifier(),
                                threshold='mean',    # return all features with value greater than the mean
                                prefit=False        # will refit
                                ).fit(X_train,y_train)

X_train.columns[sfm_rf.get_support()]

sfm_rf = SelectFromModel(RandomForestClassifier(),threshold='mean')
X_train_subset = sfm_rf.fit_transform(X_train,y_train)
X_test_subset = sfm_rf.transform(X_test)
```

Feature Selection: SelectFromModel Cont.

```
In [41]: sfm_rf = SelectFromModel(RandomForestClassifier(),
                                threshold='mean',  # return all features with value greater than the mean
                                prefit=False      # will refit
                                ).fit(X_train,y_train)

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sfm_rf = SelectFromModel(RandomForestClassifier(),threshold='mean')
X_train_subset = sfm_rf.fit_transform(X_train,y_train)
X_test_subset = sfm_rf.transform(X_test)
```

```
In [42]: sfm_rf.estimator_.feature_importances_.mean()
```

```
Out[42]: 0.07692307692307693
```

Feature Selection: SelectFromModel Cont.

```
In [41]: sfm_rf = SelectFromModel(RandomForestClassifier(),
                                threshold='mean',  # return all features with value greater than the mean
                                prefit=False      # will refit
                                ).fit(X_train,y_train)

X_train.columns[sfm_rf.get_support()]

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X_train_subset = sfm_rf.fit_transform(X_train,y_train)
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```

```
In [42]: sfm_rf.estimator_.feature_importances_.mean()
```

```
Out[42]: 0.07692307692307693
```

```
In [43]: feature_importances = pd.Series(sfm_rf.estimator_.feature_importances_,index=X_train.columns)
feature_importances.sort_values(ascending=False).round(3)
```

```
Out[43]: proline          0.284
          alcohol         0.229
          color_intensity 0.157
          flavanoids       0.101
          total_phenols    0.058
          magnesium       0.057
          alkalinity_of_ash 0.048
          od280/od315_of_diluted_wines 0.015
          nonflavanoid_phenols 0.014
          ash             0.010
          hue             0.010
          proanthocyanins  0.009
          malic_acid       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

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

```
In [44]: from sklearn.feature_selection import SelectKBest, f_classif

# select 2 best features
kbest = SelectKBest(score_func=f_classif, # default,
                    k=3,                  # how many features to keep
                    ).fit(X_train, y_train)
list(X_wine.columns[kbest.get_support()])
```

```
Out[44]: ['alcohol', 'color_intensity', 'proline']
```

Feature Selection: Recursive Feature Elimination

- Would like to test all possible combinations of features
- Likely prohibitively expensive/time-consuming
- Instead recursively select smaller subsets of features
- Requires a model that assigns weights or importance to features

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- Likely prohibitively expensive/time-consuming
- Instead recursively select smaller subsets of features
- Requires a model that assigns weights or importance to features

```
In [45]: from sklearn.feature_selection import RFE

rfe = RFE(LogisticRegression(penalty='none'), # turn of regularization
          n_features_to_select=3,             # number of feature to retain
          step=1                             # number of features to eliminate each round
          ).fit(X_train,y_train)

X_train.columns[rfe.get_support()]
```

```
Out[45]: Index(['alcohol', 'alcalinity_of_ash', 'proline'], dtype='object')
```

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`
- Exhaustive 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?

Changing number of features: Use Adjusted R^2

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- Adding features guarantees an increase in R^2
- 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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$$R^2_{adj} = 1 - (1 - R^2) \frac{n - 1}{n - m - 1}$$

- 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)
```

Changing number of features: Use Adjusted R^2 Cont.

Changing number of features: Use Adjusted R^2 Cont.

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

X_r = X_train.iloc[:,1:]
y_r = X_train.iloc[:,0] # predict alcohol from other features

lr = LinearRegression()
print(lr.fit(X_r.iloc[:, :3], y_r).score(X_r.iloc[:, :3], y_r))
print(lr.fit(X_r.iloc[:, :], y_r).score(X_r.iloc[:, :], y_r))
```

```
0.3940307310415285
0.7455685143343734
```

Changing number of features: Use Adjusted R^2 Cont.

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X_r = X_train.iloc[:,1:]
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Is this due to a better model or just adding features?

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```

```
0.3940307310415285
0.7455685143343734
```

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

```
In [48]: print(adj_r2(lr.fit(X_r.iloc[:, :3], y_r), X_r.iloc[:, :3], y_r))
print(adj_r2(lr.fit(X_r.iloc[:, :], y_r), X_r.iloc[:, :], y_r))
```

```
0.3744833352686746
0.7092211592392839
```

Changing number of features: Use Adjusted R^2 Cont.

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```

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0.3940307310415285
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print(adj_r2(lr.fit(X_r.iloc[:, :], y_r), X_r.iloc[:, :], y_r))
```

```
0.3744833352686746
0.7092211592392839
```

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

Changing number of features: Use Adjusted R^2 Cont.

Changing number of features: Use Adjusted R^2 Cont.

In [49]: `from statsmodels.api import OLS`

```
model = OLS(y_r,X_r).fit()  
print(model.rsquared_adj)  
model.summary()
```

0.709648775181579

Out[49]: OLS Regression Results

Dep. Variable:	alcohol	R-squared (uncentered):	0.746
Model:	OLS	Adj. R-squared (uncentered):	0.710
Method:	Least Squares	F-statistic:	20.76
Date:	Mon, 15 Nov 2021	Prob (F-statistic):	2.12e-20
Time:	14:22:21	Log-Likelihood:	-71.254
No. Observations:	97	AIC:	166.5
Df Residuals:	85	BIC:	197.4
Df Model:	12		
Covariance Type:	nonrobust		

	coef	std err	t	P> t	[0.025	0.975]
malic_acid	0.1412	0.064	2.201	0.030	0.014	0.269
ash	-0.0380	0.080	-0.473	0.637	-0.197	0.122
alcalinity_of_ash	-0.0283	0.082	-0.347	0.730	-0.191	0.134
magnesium	0.1268	0.072	1.763	0.081	-0.016	0.270
total_phenols	-0.1925	0.116	-1.665	0.100	-0.422	0.037
flavanoids	0.2984	0.149	1.996	0.049	0.001	0.596
nonflavanoid_phenols	-0.0106	0.087	-0.122	0.903	-0.183	0.162
proanthocyanins	-0.1724	0.076	-2.257	0.027	-0.324	-0.021
color_intensity	0.3969	0.116	3.423	0.001	0.166	0.627
hue	-0.0260	0.064	-0.410	0.683	-0.152	0.100

Questions re Adjusted 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

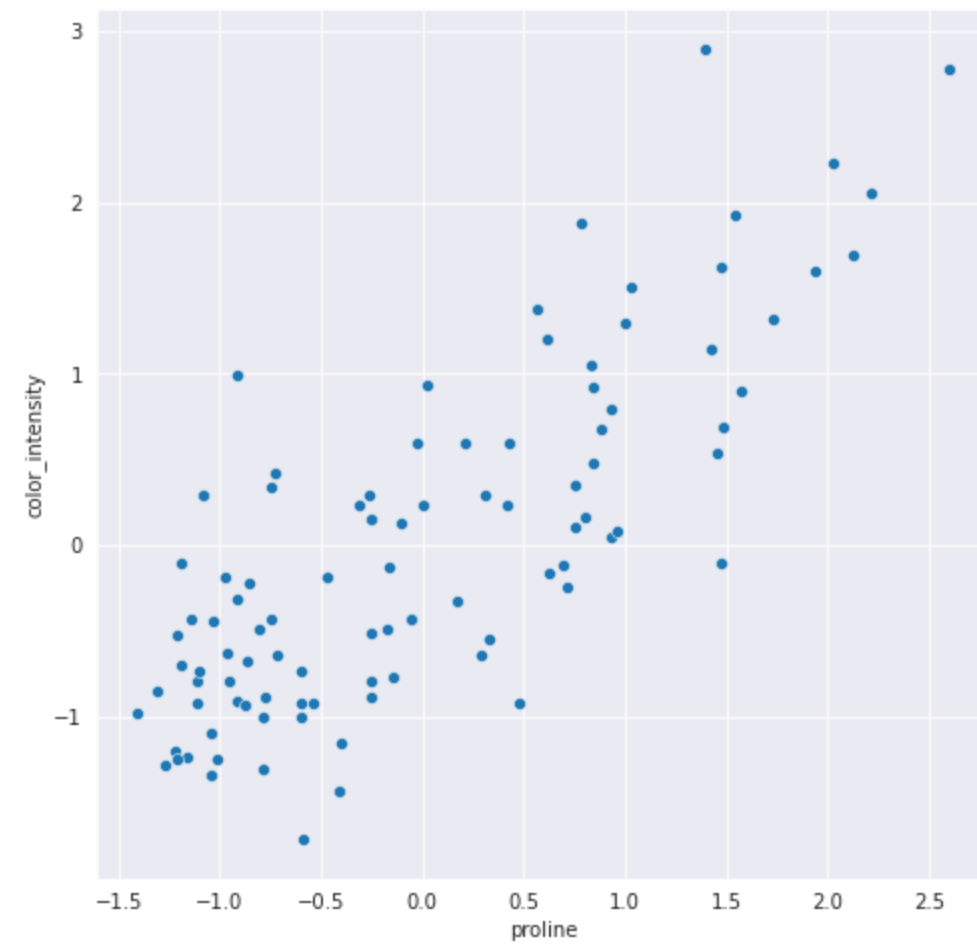
Principal Component Analysis (PCA)

- How it works:
 0. first center the data (subtract the means)
 1. first component:
 - direction (combination of features)
 - explains maximum variance
 2. 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

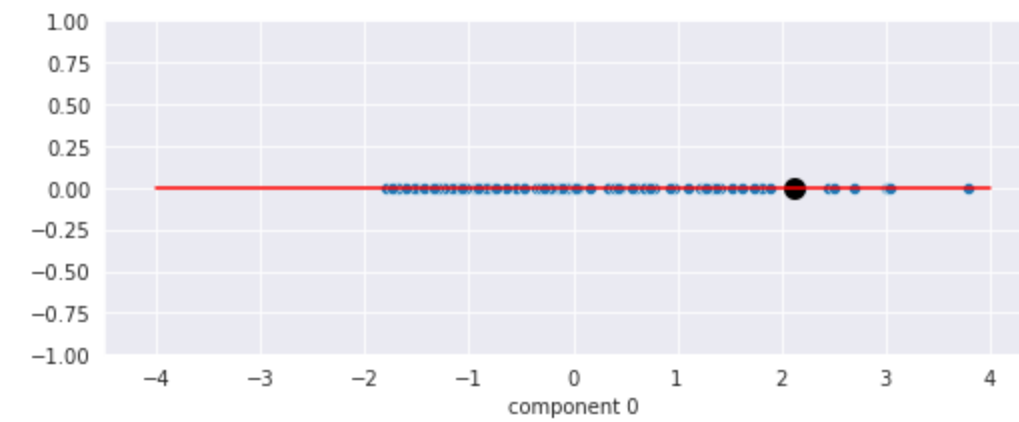
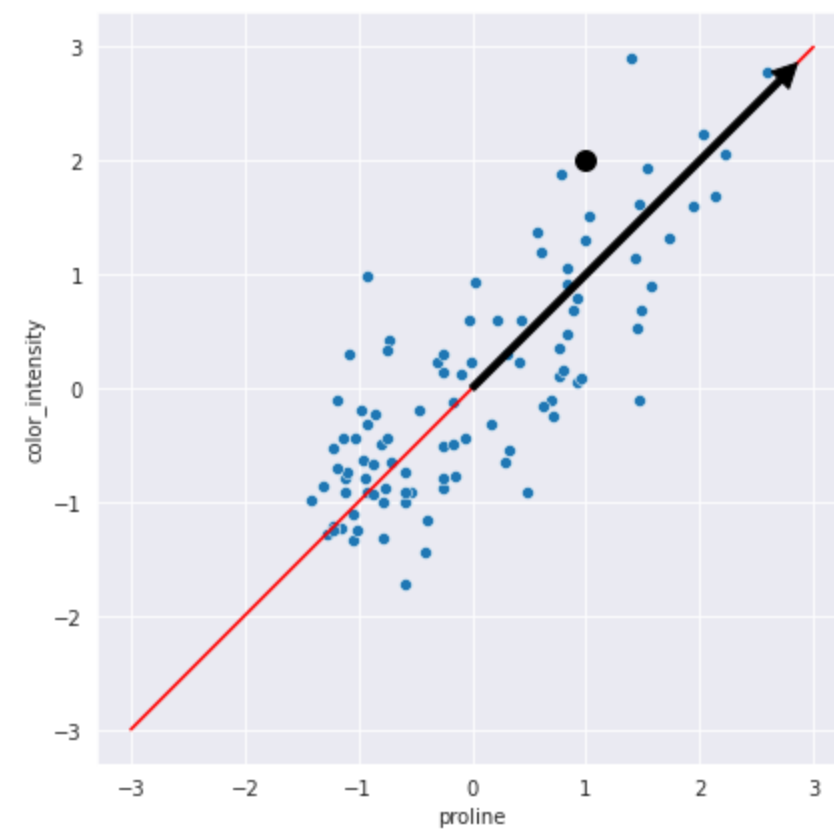
```
In [51]: fig, ax = plt.subplots(1, 1, figsize=(8, 8))  
sns.scatterplot(x='proline', y='color_intensity', data=X_train, ax=ax);
```



PCA Example Cont.

PCA Example Cont.

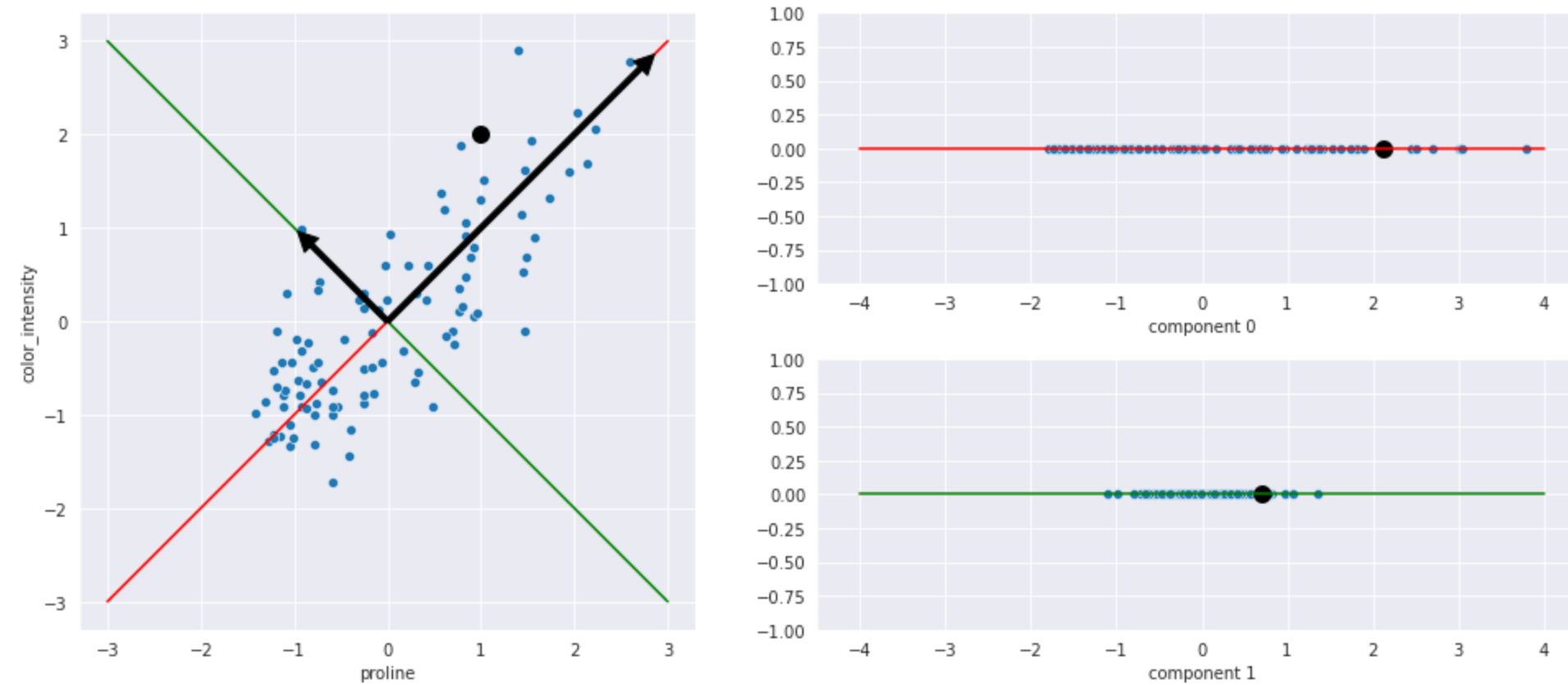
```
In [53]: plot_pca(X_train[['proline', 'color_intensity']],pca,num_components=1)  
plt.tight_layout()
```



PCA Example Cont.

PCA Example Cont.

```
In [54]: plot_pca(X_train[['proline', 'color_intensity']],pca,num_components=2)  
plt.tight_layout()
```



PCA in sklearn

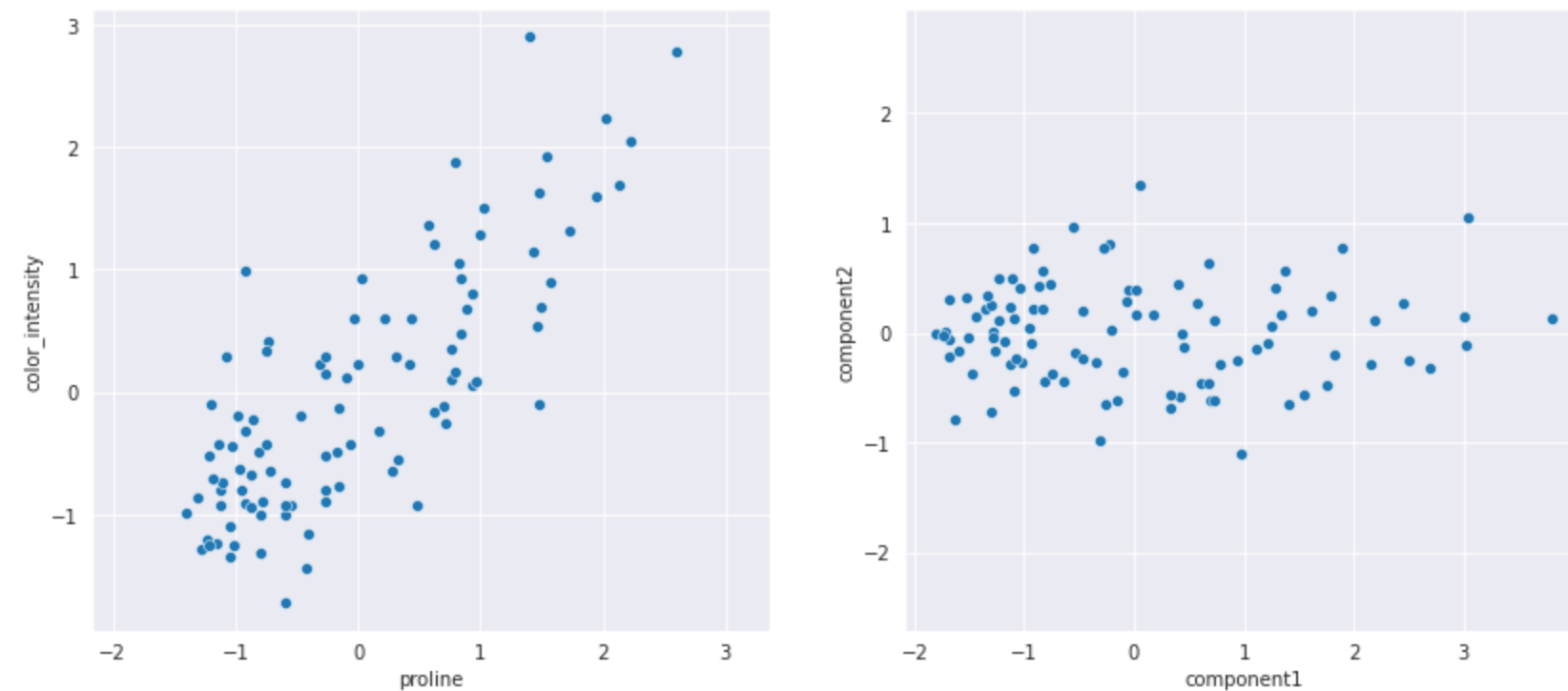
PCA in sklearn

```
In [55]: from sklearn.decomposition import PCA

# extract the first 2 principle compenents
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_train[['proline', 'color_intensity']])

X_pca = pd.DataFrame(X_pca, columns=['component1', 'component2'])

fig, ax=plt.subplots(1,2,figsize=(14,6))
sns.scatterplot(x='proline', y='color_intensity', data=X_train, ax=ax[0]);
sns.scatterplot(x='component1', y='component2', data=X_pca, ax=ax[1]);
ax[0].axis('equal'); ax[1].axis('equal');
```



PCA: Explained Variance

- How much of the variance is explained by each component?

PCA: Explained Variance

- How much of the variance is explained by each component?

```
In [56]: pca.explained_variance_ratio_
```

```
Out[56]: array([0.89808764, 0.10191236])
```

PCA: Principle Components

- What does the first component (vector) look like?

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```
In [57]: pca.components_[0]
```

```
Out[57]: array([0.70710678, 0.70710678])
```

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In [57]: pca.components_[0]
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- And the second?

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```

- And the second?

```
In [58]: pca.components_[1]
```

```
Out[58]: array([-0.70710678, 0.70710678])
```

PCA: Principle Components

- What does the first component (vector) look like?

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In [57]: pca.components_[0]
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```

- All components returned

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In [58]: pca.components_[1]
```

```
Out[58]: array([-0.70710678, 0.70710678])
```

- All components returned

```
In [59]: pca.components_
```

```
Out[59]: array([[ 0.70710678,  0.70710678],  
                [-0.70710678,  0.70710678]])
```


PCA: Principle Components

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- And the second?

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```
In [59]: pca.components_
```

```
Out[59]: array([[ 0.70710678,  0.70710678],  
                [-0.70710678,  0.70710678]])
```

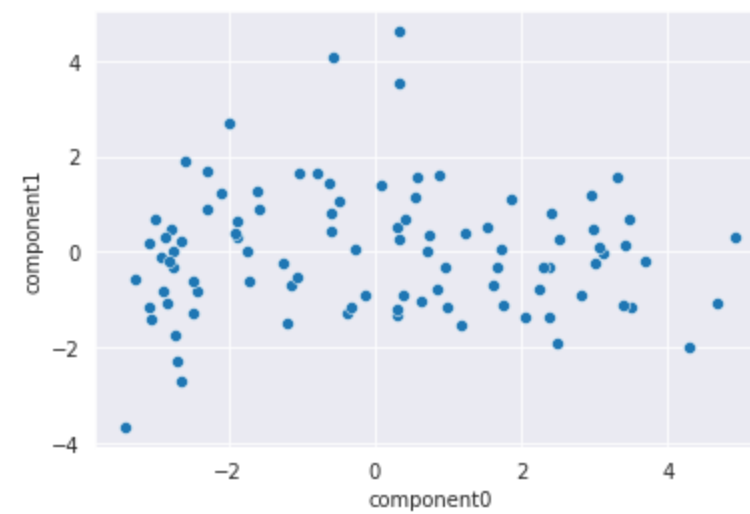
```
In [60]: # Can also return the singular values themselves  
pca.singular_values_
```

```
Out[60]: array([13.1995834 ,  4.44645904])
```

Dimensionality Reduction with PCA

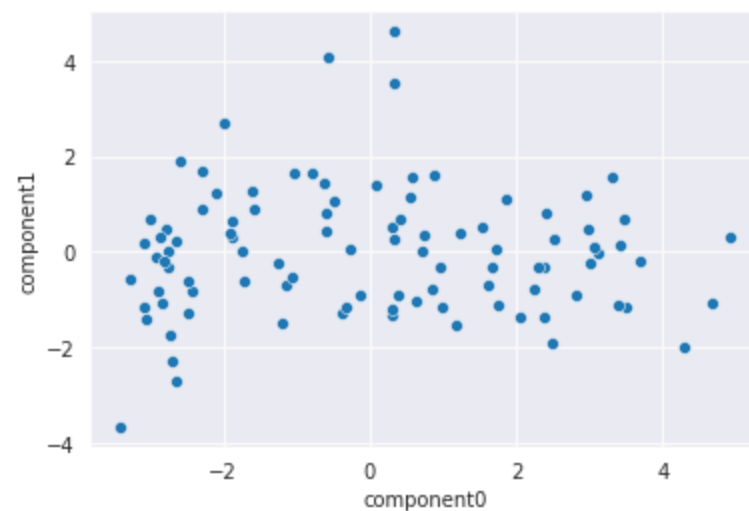
Dimensionality Reduction with PCA

```
In [61]: pca_2d = PCA(n_components=2)
X_2d = pca_2d.fit_transform(X_train)
X_2d = pd.DataFrame(X_2d, columns=["component"+str(i) for i in range(2)])
sns.scatterplot(x='component0', y='component1', data=X_2d);
```



Dimensionality Reduction with PCA

```
In [61]: pca_2d = PCA(n_components=2)
X_2d = pca_2d.fit_transform(X_train)
X_2d = pd.DataFrame(X_2d, columns=["component"+str(i) for i in range(2)])
sns.scatterplot(x='component0', y='component1', data=X_2d);
```



```
In [62]: print(' + \n'.join([f'{w: 0.2f}*{f}' for f,w in sorted(zip(X_train.columns,pca_2d.components_[0]),key=lambda x:x[1])]))

-0.28*nonflavanoid_phenols +
-0.26*alcalinity_of_ash +
-0.03*hue +
 0.01*malic_acid +
 0.11*ash +
 0.21*proanthocyanins +
 0.23*magnesium +
 0.25*od280/od315_of_diluted_wines +
 0.36*proline +
 0.36*color_intensity +
 0.36*total_phenols +
 0.37*alcohol +
 0.39*flavanoids
```

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)
- 1024×1024 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 Faces recognition example using eigenfaces and SVMs

Example Dataset: Labeled Faces in the Wild (LFW)

Labeled Faces in the Wild

Example Dataset: Labeled Faces in the Wild (LFW)

Labeled Faces in the Wild

```
In [64]: from sklearn.datasets import fetch_lfw_people  
         lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)
```


Example Dataset: Labeled Faces in th Wild (LFW)

Labeled Faces in the Wild

```
In [64]: from sklearn.datasets import fetch_lfw_people  
  
lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)
```

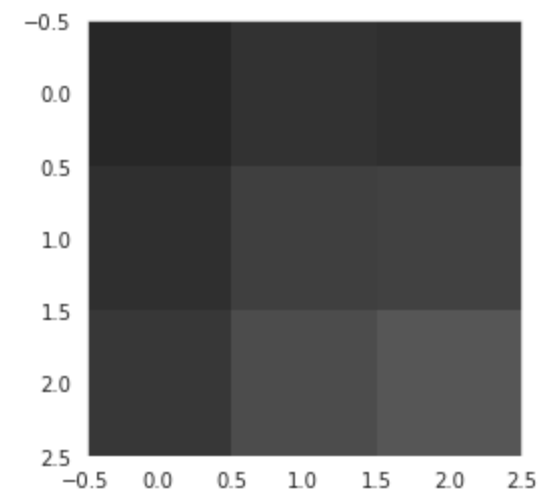
```
In [65]: sns.set_style('dark')  
plt.imshow(lfw_people.images[1], cmap=plt.cm.gray, vmin=0, vmax=255)  
plt.title(lfw_people.target_names[lfw_people.target[1]], size=12);
```



Example Pixel Values

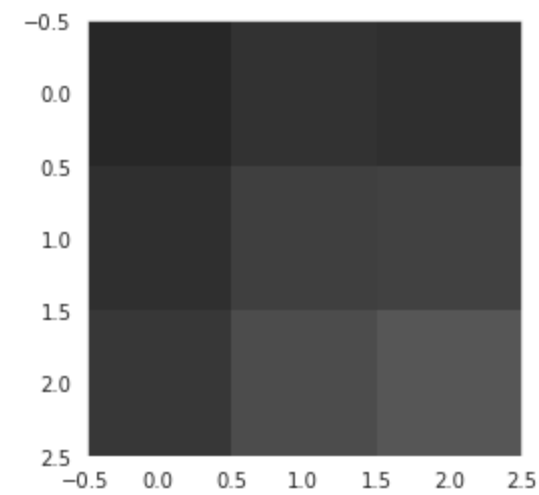
Example Pixel Values

```
In [66]: # first 3x3 set of pixels  
plt.imshow(lfw_people.images[1][:3,:3],cmap=plt.cm.gray,vmin=0, vmax=255);
```



Example Pixel Values

```
In [66]: # first 3x3 set of pixels
plt.imshow(lfw_people.images[1][:3,:3],cmap=plt.cm.gray,vmin=0, vmax=255);
```



```
In [67]: lfw_people.images[1][:3,:3]
```

```
Out[67]: array([[39.666668, 50.333332, 47.        ],
                [47.666668, 63.        , 65.333336],
                [55.333332, 76.666664, 86.333336]], dtype=float32)
```

Representing each Image: Flatten

- Grid as a fixed length feature vector?

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```
In [68]: lfw_people.images[1].shape
```

```
Out[68]: (50, 37)
```

Representing each Image: Flatten

- Grid as a fixed length feature vector?

```
In [68]: lfw_people.images[1].shape
```

```
Out[68]: (50, 37)
```

```
In [69]: x = lfw_people.images[1].reshape(1, -1)  
x
```

```
Out[69]: array([[ 39.666668,  50.333332,  47.          , ..., 117.666664, 115.          ,  
                  133.66667  ]], dtype=float32)
```

Representing each Image: Flatten

- Grid as a fixed length feature vector?

```
In [68]: lfw_people.images[1].shape
```

```
Out[68]: (50, 37)
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```

```
In [70]: x.shape
```

```
Out[70]: (1, 1850)
```


Representing each Image: Flatten

- Grid as a fixed length feature vector?

```
In [68]: lfw_people.images[1].shape
```

```
Out[68]: (50, 37)
```

```
In [69]: x = lfw_people.images[1].reshape(1, -1)  
x
```

```
Out[69]: array([[ 39.666668,  50.333332,  47.          , ..., 117.666664, 115.          ,  
                133.66667 ]], dtype=float32)
```

```
In [70]: x.shape
```

```
Out[70]: (1, 1850)
```

What information do we lose when we do this?

Create a Dataset

Create a Dataset

```
In [71]: # 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=123)

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: 50x37
n_features: 1850
n_classes : 7
n_train   : 966
n_test    : 322
```

Compute PCA and Transform

Compute PCA and Transform

```
In [72]: # set the number of dimensions we want to retain
n_components = 150

# 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_pca_faces = pca_faces.transform(X_train_faces)
X_test_pca_faces = pca_faces.transform(X_test_faces)
```

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```

```
In [73]: pca_faces.components_[0]
```

```
Out[73]: array([-0.01278668, -0.01292658, -0.01463957, ..., -0.00385124,
               -0.00411337, -0.0045574 ], dtype=float32)
```

Compute PCA and Transform

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```

```
In [73]: pca_faces.components_[0]
```

```
Out[73]: array([-0.01278668, -0.01292658, -0.01463957, ..., -0.00385124,
               -0.00411337, -0.0045574 ], dtype=float32)
```

```
In [74]: pca_faces.singular_values_
```

```
Out[74]: array([21388.467 , 19735.988 , 13733.558 , 12266.252 , 11349.948 ,
                8755.401 , 7928.223 , 7296.223 , 7035.028 , 6864.7207 ,
                6348.1304 , 6118.6055 , 5526.047 , 5221.793 , 4977.621 ,
                4962.2236 , 4785.6265 , 4679.6924 , 4524.9766 , 4275.846 ,
                4209.652 , 4032.5813 , 3924.0525 , 3801.2917 , 3723.4976 ,
                3675.6616 , 3581.645 , 3497.1353 , 3378.749 , 3268.003 ,
                3137.3608 , 3030.9197 , 3017.3242 , 2981.4546 , 2897.5417 ,
                2858.5464 , 2792.041 , 2762.1348 , 2726.447 , 2702.855 ,
                2661.0544 , 2591.7307 , 2543.3933 , 2526.289 , 2459.802 ,
                2429.5876 , 2417.179 , 2379.5273 , 2339.4941 , 2332.3047 ,
                2293.3118 , 2283.203 , 2221.0967 , 2194.8472 , 2160.4968 ,
```

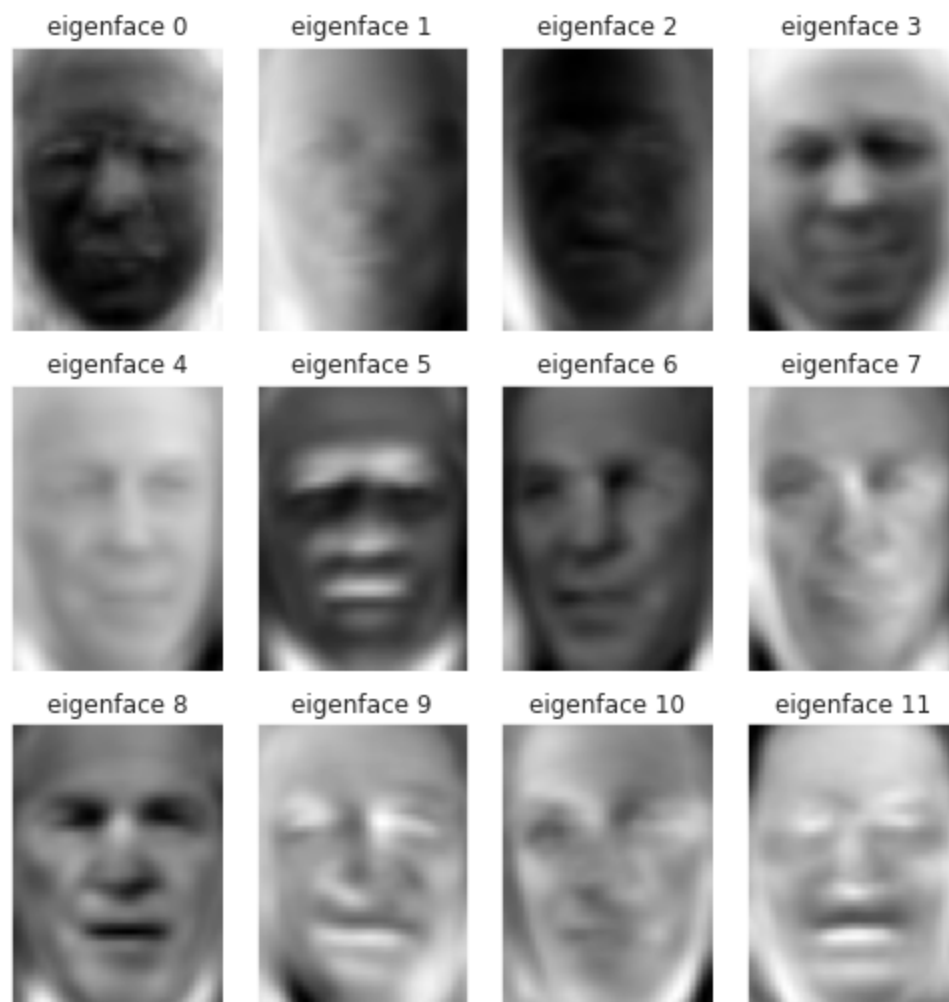
Eigenfaces

- What if we plot the top 12 components (eigenfaces) using `.reshape(h,w)`?

Eigenfaces

- What if we plot the top 12 components (eigenfaces) using `.reshape(h,w)`?

```
In [76]: eigenface_titles = ["eigenface %d" % i for i in range(eigenfaces.shape[0])]
plot_gallery(eigenfaces, eigenface_titles, h, w)
plt.tight_layout()
```



Train and Tune SVC

Train and Tune SVC

```
In [77]: %%time
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC

params = {'C': [1e3, 5e3, 1e4, 5e4, 1e5],
          'gamma': [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.1], }
clf_faces = GridSearchCV(SVC(kernel='rbf', class_weight='balanced'),
                        params, cv=3, n_jobs=-1)
clf_faces = clf_faces.fit(X_train_pca_faces, y_train_faces)
```

```
CPU times: user 258 ms, sys: 133 ms, total: 391 ms
Wall time: 2.71 s
```

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clf_faces = clf_faces.fit(X_train_pca_faces, y_train_faces)
```

```
CPU times: user 258 ms, sys: 133 ms, total: 391 ms
Wall time: 2.71 s
```

```
In [78]: print(f"best_params : {clf_faces.best_params_}")
print(f"best_score : {clf_faces.best_score_:0.2f}")
```

```
best_params : {'C': 1000.0, 'gamma': 0.005}
best_score  : 0.79
```

Evaluate on the test set

Evaluate on the test set

```
In [79]: y_pred = clf_faces.predict(X_test_pca_faces)
         from sklearn.metrics import classification_report
         print(classification_report(y_test_faces, y_pred, target_names=target_names))
```

	precision	recall	f1-score	support
Ariel Sharon	0.93	0.74	0.82	19
Colin Powell	0.82	0.86	0.84	59
Donald Rumsfeld	0.89	0.83	0.86	30
George W Bush	0.84	0.97	0.90	133
Gerhard Schroeder	1.00	0.52	0.68	27
Hugo Chavez	1.00	0.61	0.76	18
Tony Blair	0.84	0.89	0.86	36
accuracy			0.86	322
macro avg	0.90	0.77	0.82	322
weighted avg	0.87	0.86	0.85	322

Prediction Examples

Prediction Examples

```
In [80]: prediction_titles = [title(y_pred, y_test_faces, target_names, i)
                                for i in range(y_pred.shape[0])]

plot_gallery(X_test_faces, prediction_titles, h, w)
plt.tight_layout()
```



Performance without PCA

Performance without PCA

```
%%time

# Warning: this cell takes up to 2 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 = GridSearchCV(SVC(kernel='rbf', class_weight='balanced'),
                          params, cv=3, n_jobs=-1)
clf_faces = clf_faces.fit(X_train_faces, y_train_faces)

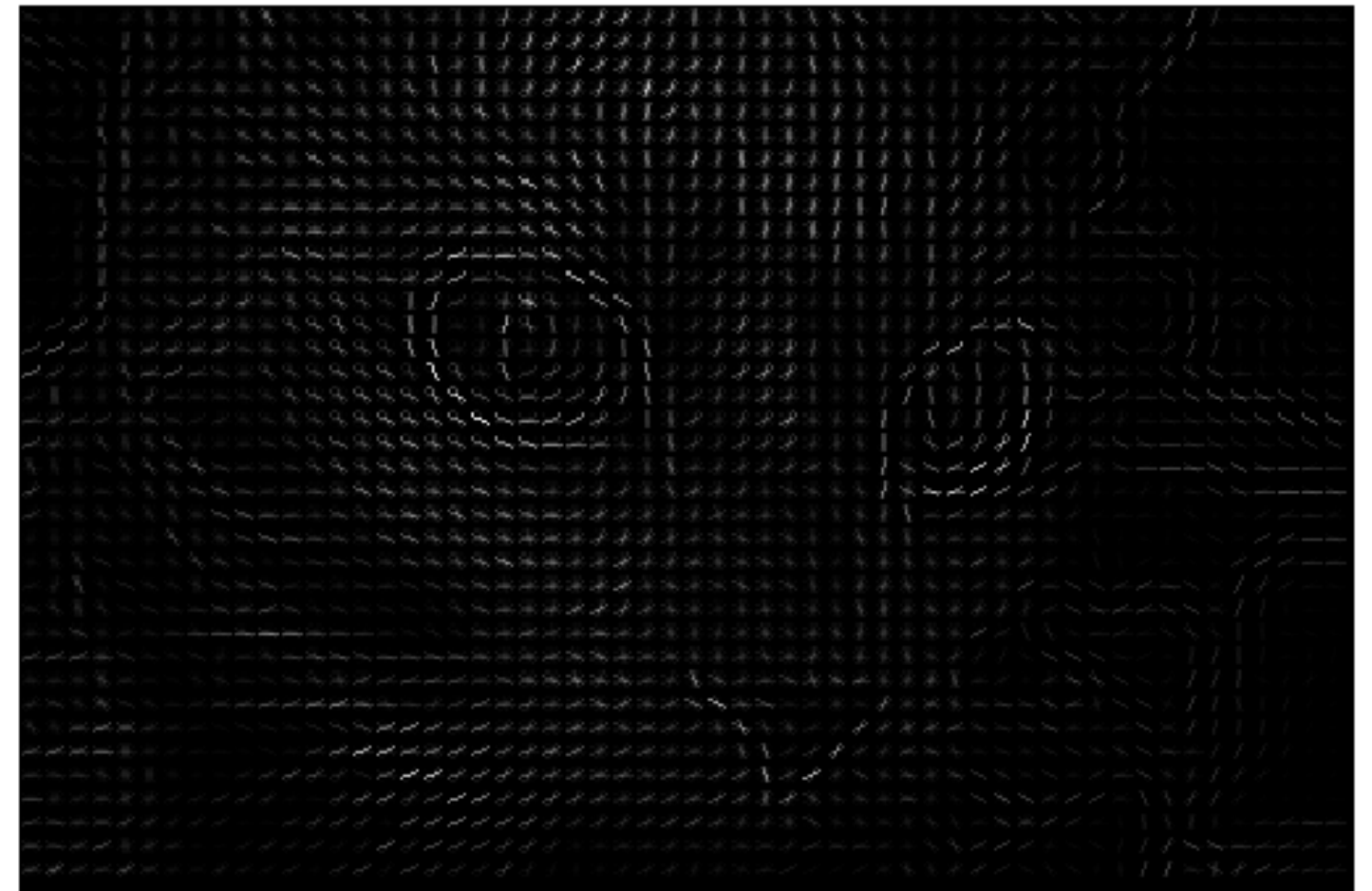
# CPU times: user 9.57 s, sys: 72.1 ms, total: 9.64 s
# Wall time: 1min 18s

print(f"best_params : {clf_faces.best_params_}")
print(f"best_score   : {clf_faces.best_score_:0.2f}")

# best_params : {'C': 1000.0, 'gamma': 0.0001}
# best_score   : 0.41
```

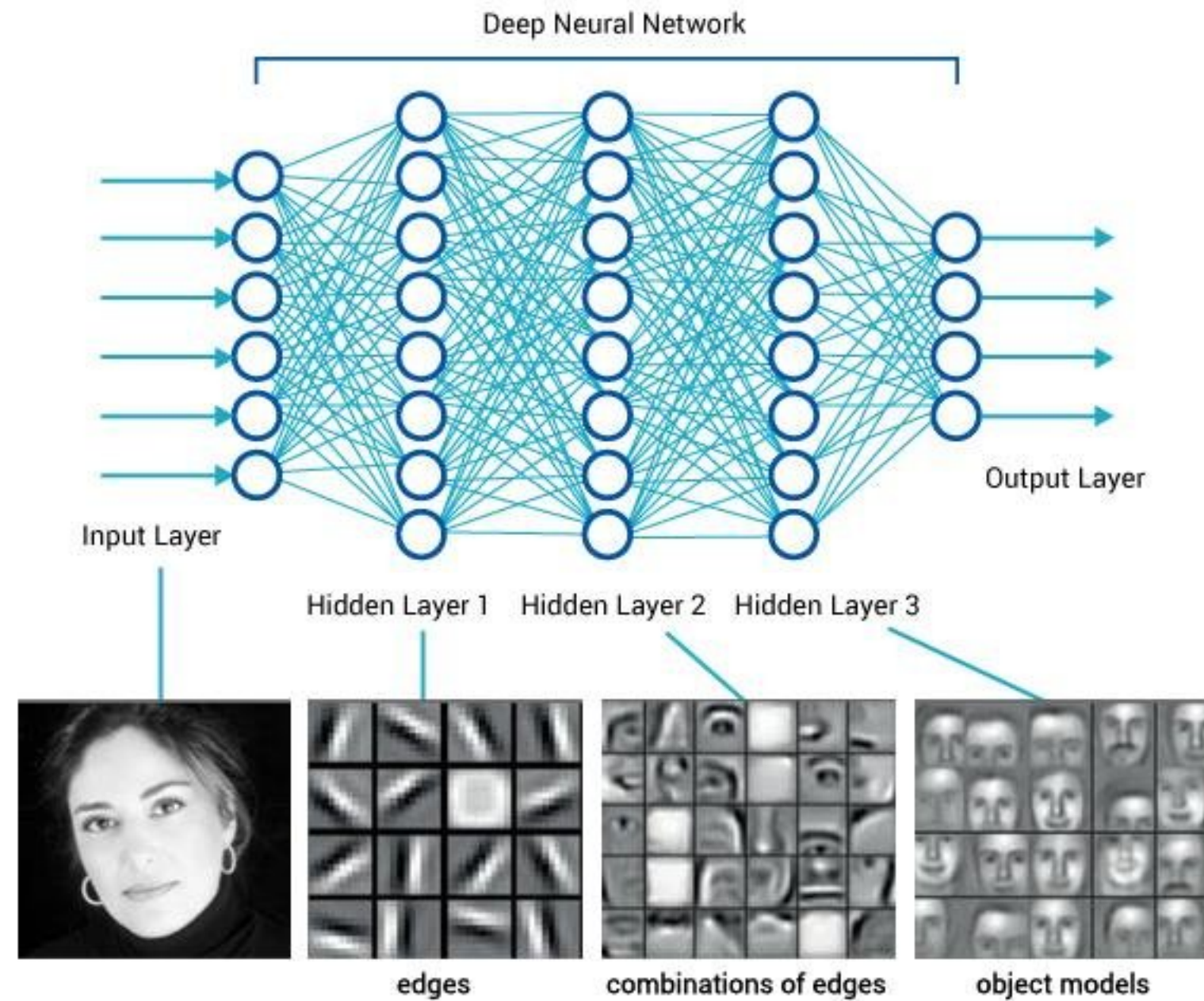
Other Image Recognition Methods

- With Feature Engineering and general models
 - ex: Histogram of Oriented Gradients or HOG (See [PDSH Chap 5](#))
 - many more (See [scikit-image](#))



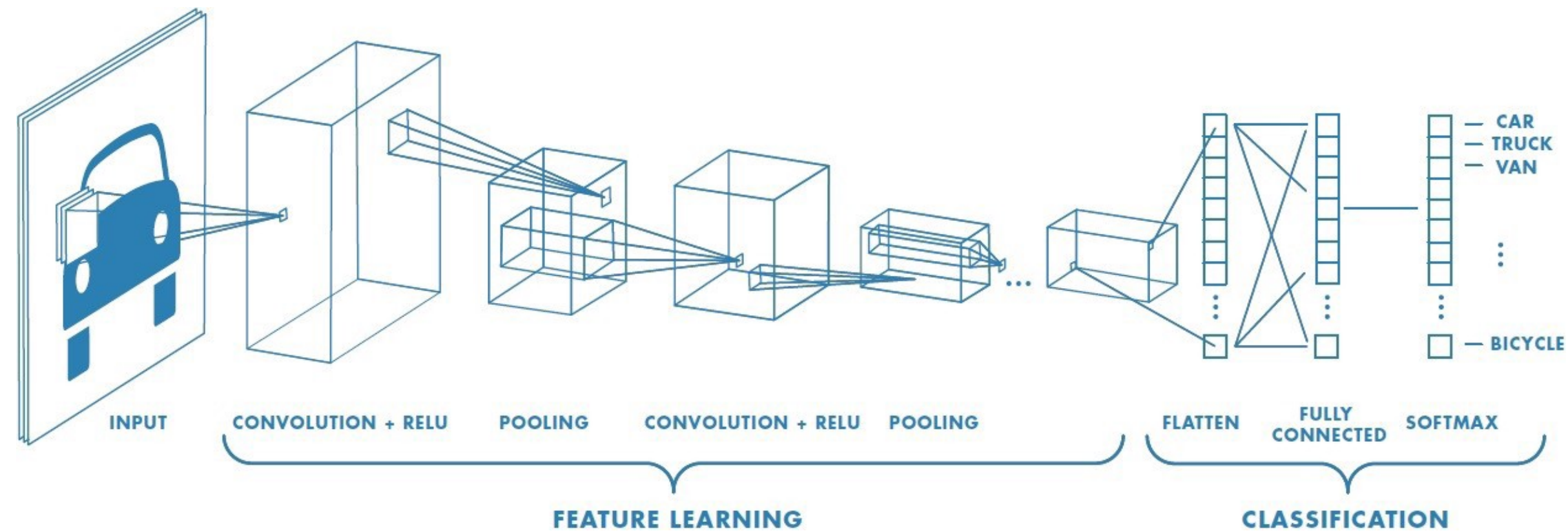
Other Image Recognition Methods: Deep Neural Networks

- With Deep Neural Nets



Other Image Recognition Methods: Deep Neural Networks

- With Convolutional Neural Networks [Good Example](#)



From <https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53>

Questions re Feature Extraction and PCA?

Next time: NLP and Pipelines