Elements Of Data Science - F2020

Week 9: Dimensionality Reduction, Feature Selection and Feature Extraction

11/16/2020

TODOs

- Readings:
    - PML Chapter 6, first 3 sections on Pipelines
    - PML Chapter 8
- HW3, Out this week
- Answer and submit Quiz 9, **Sunday Nov 22nd, 11:59pm ET**

Today

- **Joining Datasets**
- **Dimensionality Reduction**
    - **Feature Selection**
        - LASSO
        - Tree Based Models Feature Importance
        - Univariate Tests
        - Recursive Feature Selection
    - **Feature Extraction**
        - PCA
- **Image Recognition Using PCA**

Questions?

Simple Joins: Sharing An Index

In [2]:
```
df1 = pd.DataFrame({'A': ['A0','A1','A2']})
df1
```

Out[2]:

	A
0	A0
1	A1
2	A2

In [3]:
```
df2 = pd.DataFrame({'B': ['B0','B1','B2']})
df2
```

Out[3]:

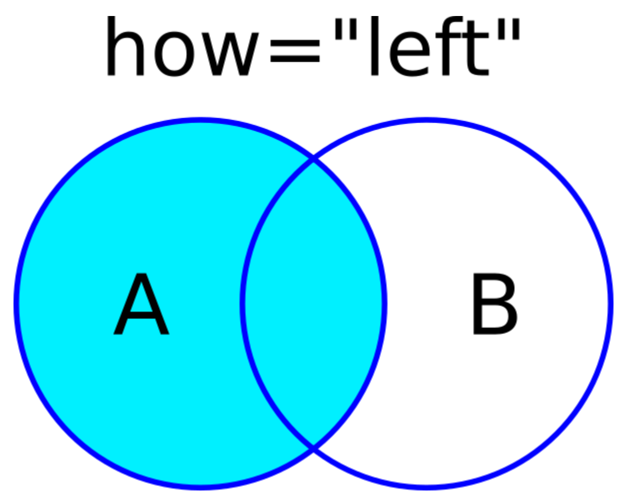
	B
0	B0
1	B1
2	B2

In [4]:
```
df1.join(df2)
```

Out[4]:

	A	B
0	A0	B0
1	A1	B1
2	A2	B2

Simple Joins: Left Join



In [5]:
```
df3 = pd.DataFrame({'C': ['C1','C2','C3']},index=[1,2,3])
df3
```

Out[5]:

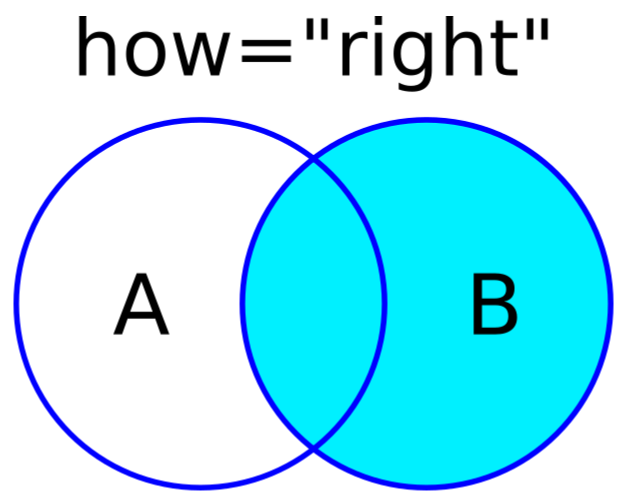
	C
1	C1
2	C2
3	C3

In [6]:
```
df1.join(df3,how="left") # default is left join
```

Out[6]:

	A	C
0	A0	NaN
1	A1	C1
2	A2	C2

Simple Joins: Right Join

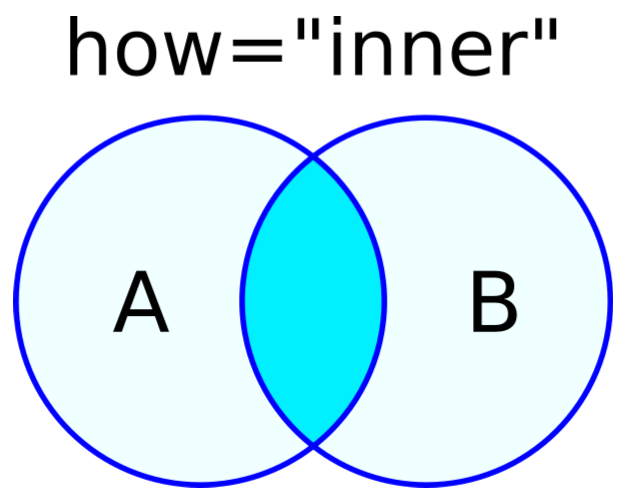


```
In [7]: df1.join(df3,how="right")

Out[7]:
```

	A	C
1	A1	C1
2	A2	C2
3	NaN	C3

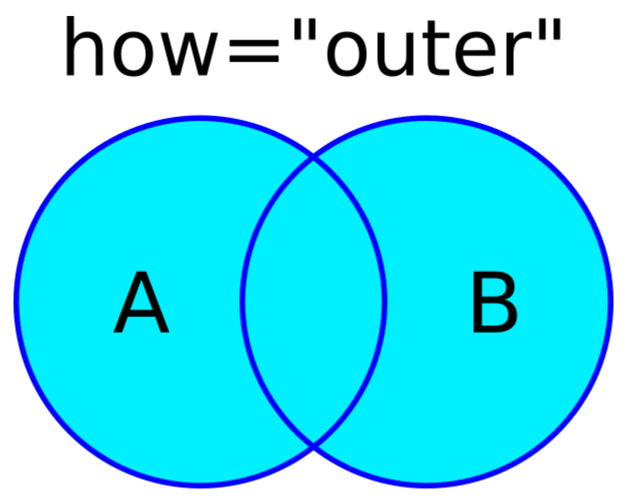
Simple Joins: Inner Join

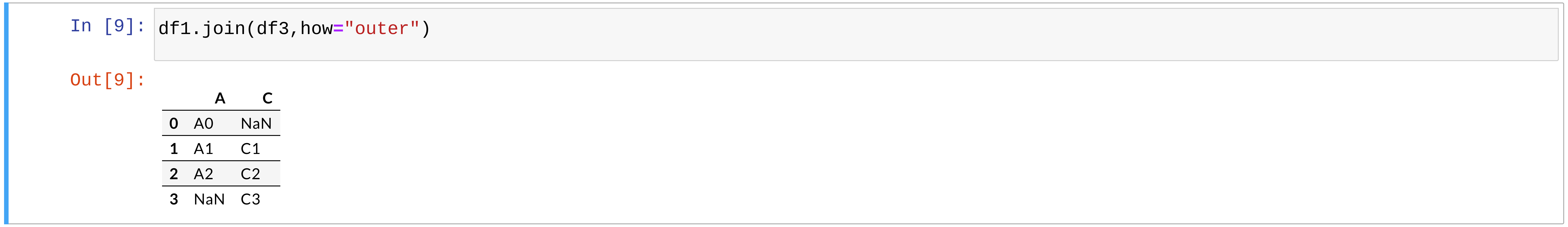


```
In [8]: df1.join(df3,how="inner")
```

```
Out[8]:
      A   C
1    A1  C1
2    A2  C2
```

Simple Joins: Outer Join





```
In [9]: df1.join(df3,how="outer")
```

Out[9]:

	A	C
0	A0	NaN
1	A1	C1
2	A2	C2
3	NaN	C3

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 modle 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 features to generate a new feature space

Load Binary Wine Classification

```
In [10]: 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
         X_wine = X_wine.iloc[y_wine < 2]
         y_wine = y_wine[y_wine < 2]
         feature_names = X_wine.columns.values
         X_train,X_test,y_train,y_test = train_test_split(X_wine,y_wine,random_state=0)
         X_train = pd.DataFrame(X_train,columns=X_wine.columns)
         feature_names
```

```
Out[10]: 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)
```

Standardize Features

In [11]:
```
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)
```

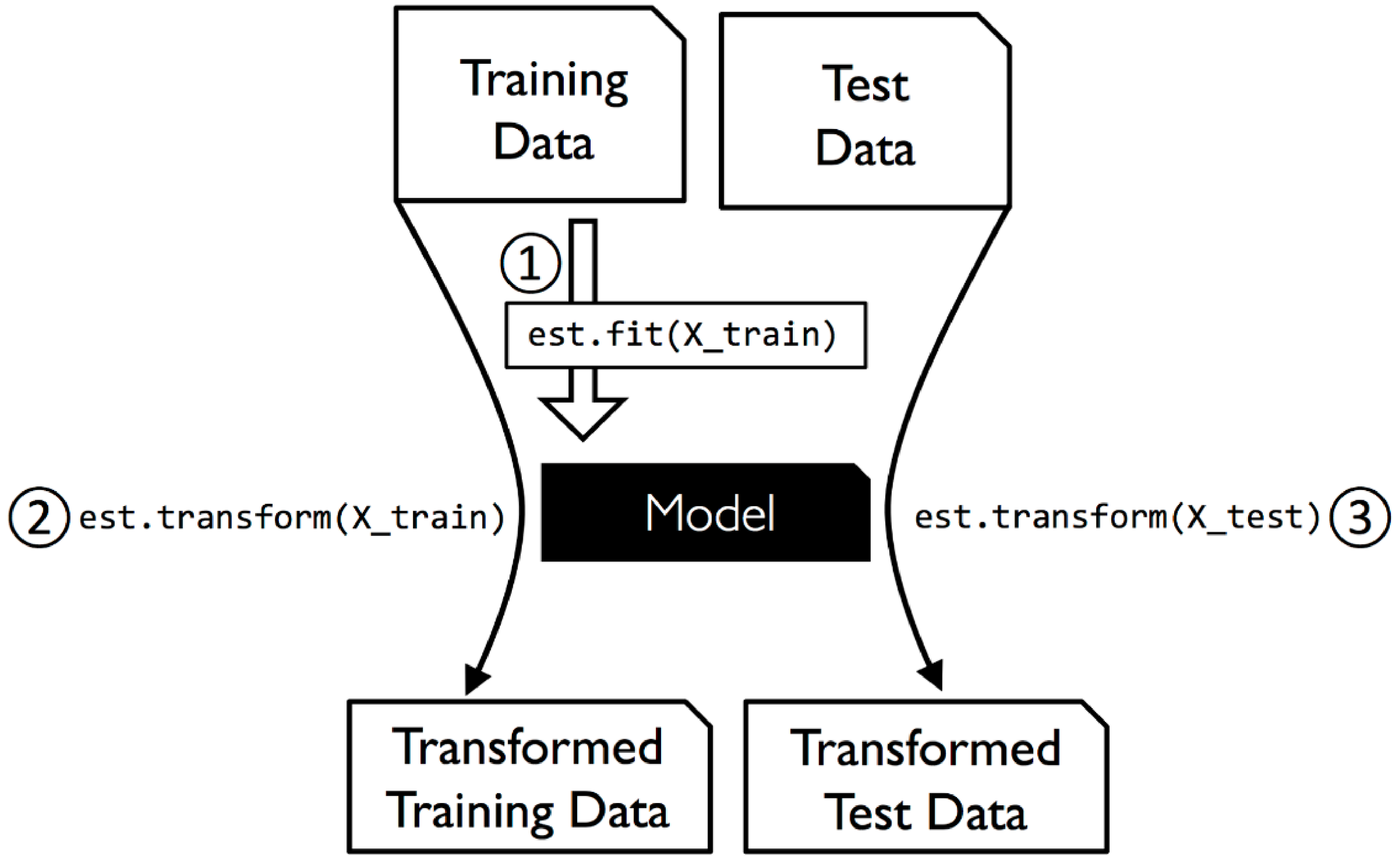
In [12]:
```
X_train.agg(['mean','std']).round(1).T.head()
```

Out[12]:

	mean	std
alcohol	0.0	1.0
malic_acid	-0.0	1.0
ash	-0.0	1.0
alcalinity_of_ash	0.0	1.0
magnesium	0.0	1.0

Aside: Predicting vs Transforming with Train/Test Split

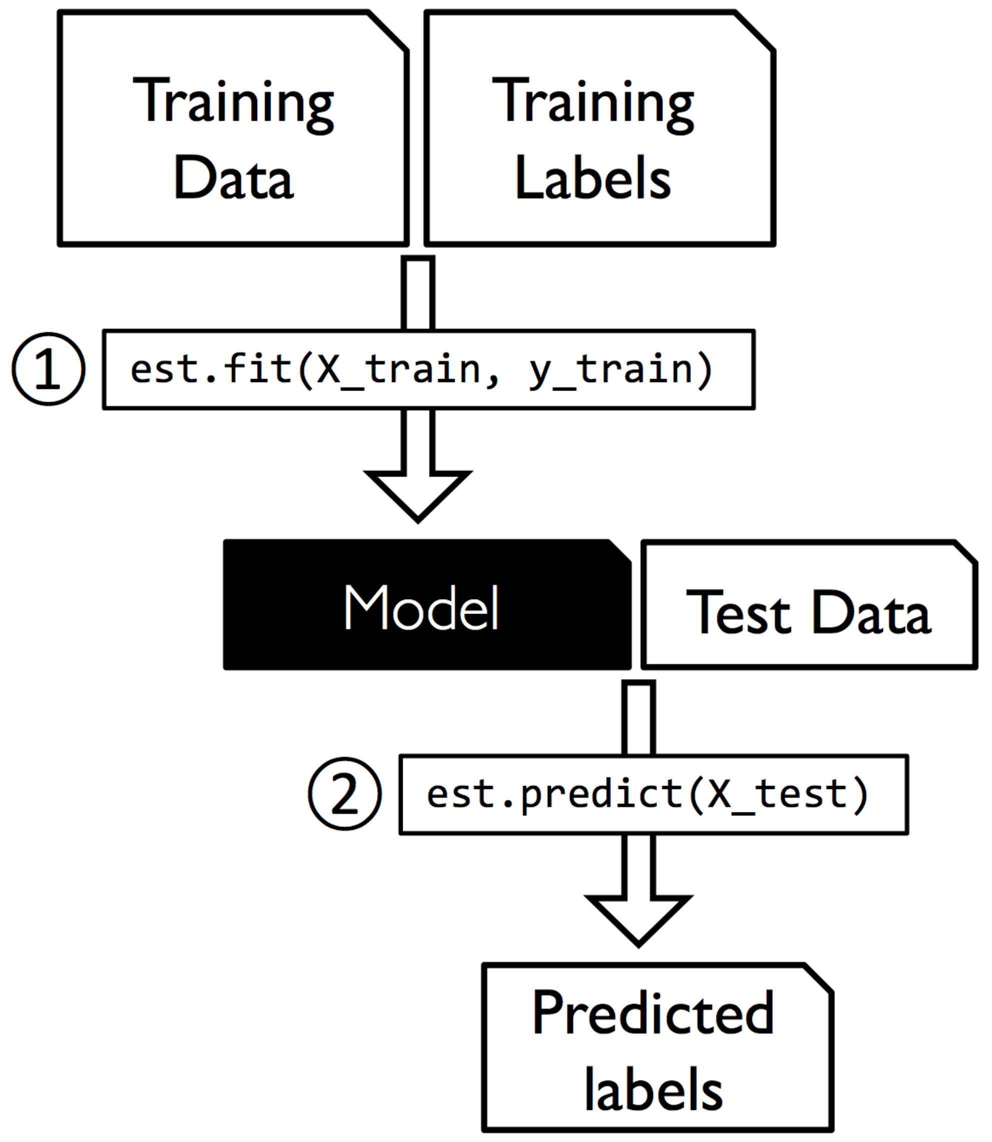
- When transforming data, fit on the training set, transform both train and test



From PML

Aside: Predicting vs Transforming with Train/Test Split

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



From PML

Feature Selection: LASSO (L1)

In [13]:
```python
from sklearn.linear_model import LogisticRegression

logr = LogisticRegression(C=100, penalty="l1", solver="liblinear", random_state=123)
logr.fit(X_train, y_train)

logr.coef_
```

Out[13]:
```
array([[-5.74709641, -1.20824931, -2.70057811,  2.47398434, -0.28304842,
        -0.14584941, -0.37559551,  0.        ,  1.14394581, -0.63815798,
         1.06926936, -0.86036347, -7.567675  ]])
```

In [14]:
```python
logr = LogisticRegression(C=0.1, penalty="l1", solver="liblinear", random_state=123)
logr.fit(X_train, y_train)
logr.coef_
```

Out[14]:
```
array([[-0.98231183,  0.        ,  0.        ,  0.        ,  0.        ,
         0.        , -0.00652705,  0.        ,  0.        ,  0.        ,
         0.        ,  0.        , -1.10166563]])
```

In [15]:
```python
feature_names[logr.coef_[0] != 0]
```

Out[15]:
```
array(['alcohol', 'flavanoids', 'proline'], dtype=object)
```

Feature Selection: Tree Based Model Feature Importance

In [16]:
```python
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
```

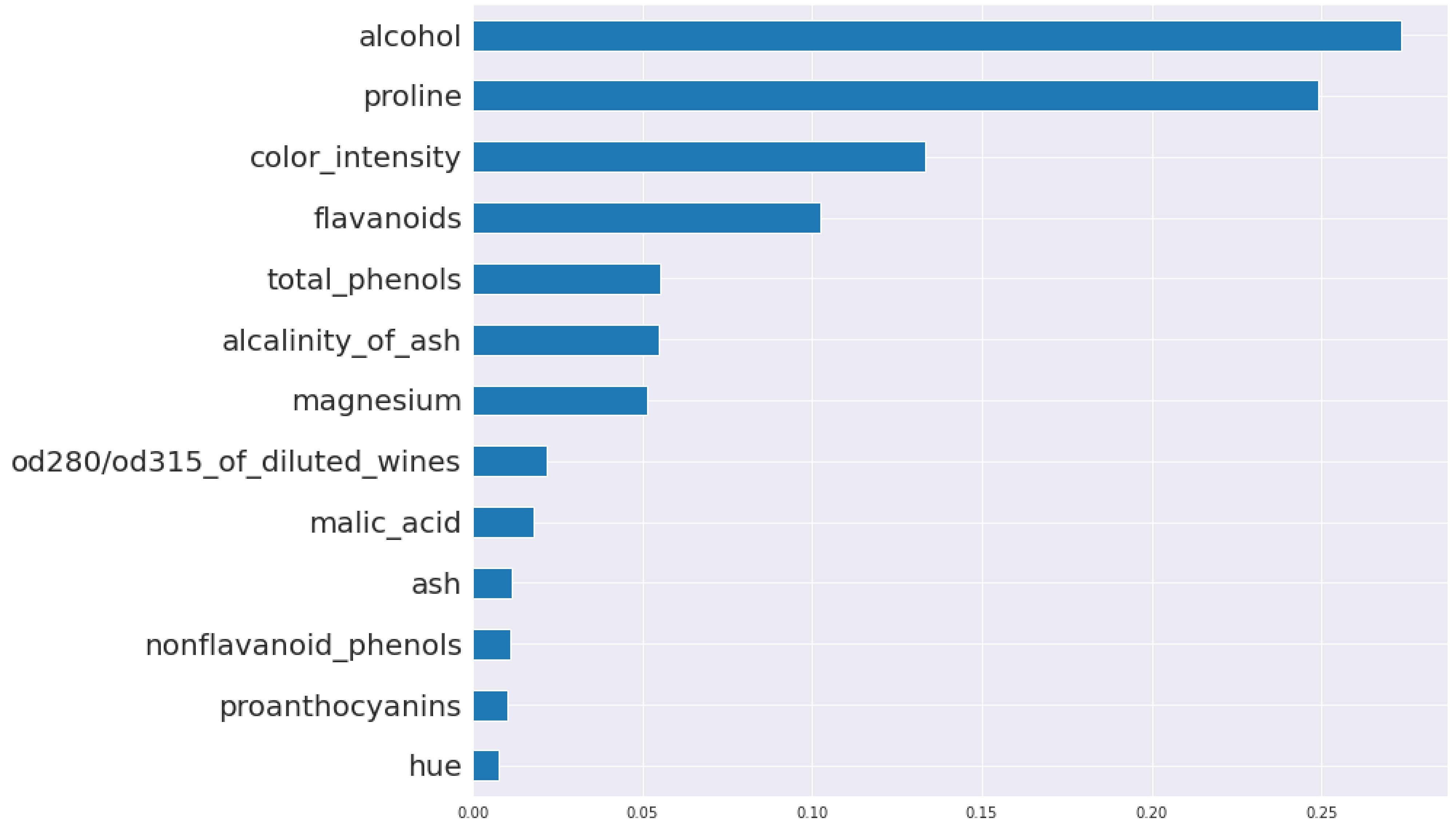
Out[16]:
```
array([0.27332426, 0.01783127, 0.01145411, 0.05480187, 0.05158374,
       0.05521824, 0.10260545, 0.01117794, 0.01033494, 0.13339066,
       0.00759636, 0.0216486 , 0.24903258])
```

In [17]:
```python
feature_importances = pd.Series(rf.feature_importances_,index=feature_names)
feature_importances.sort_values(ascending=False).round(3)
```

Out[17]:
```
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

In [18]:
```
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: SelectFromModel

```
In [19]: from sklearn.feature_selection import SelectFromModel

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

         sfm.get_support()
```

```
Out[19]: array([ True, False, False, False, False, False,  True, False, False,
                False, False, False,  True])
```

```
In [20]: feature_names[sfm.get_support()]
```

```
Out[20]: array(['alcohol', 'flavanoids', 'proline'], dtype=object)
```

```
In [21]: X_train_subset = sfm.transform(X_train)
         X_train_subset.shape
```

```
Out[21]: (97, 3)
```

```
In [22]: sfm_rf = SelectFromModel(RandomForestClassifier(),
                                  threshold='mean',   # return all features with value greater than the mean
                                  prefit=False        # need to refit
                                 ).fit(X_train,y_train)
         feature_names[sfm_rf.get_support()]
```

```
Out[22]: array(['alcohol', 'flavanoids', 'color_intensity', 'proline'],
               dtype=object)
```

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
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- Example: `f_classif`
    - F-test
    - estimates the degree of linear dependency between feature x and target y

In [23]:
```
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[23]:
```
['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

In [24]:
```
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)

feature_names[rfe.get_support()]
```

Out[24]:
```
array(['alcohol', 'alcalinity_of_ash', 'proline'], dtype=object)
```

Feature Selection: Other Methods

- by Variance
    - eliminate columns where all rows have 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
    - `chi2`, requires non-negative values
    - `f_regression`, F-test for regression task
    - `mutual_info_classif` and `_regression`

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)

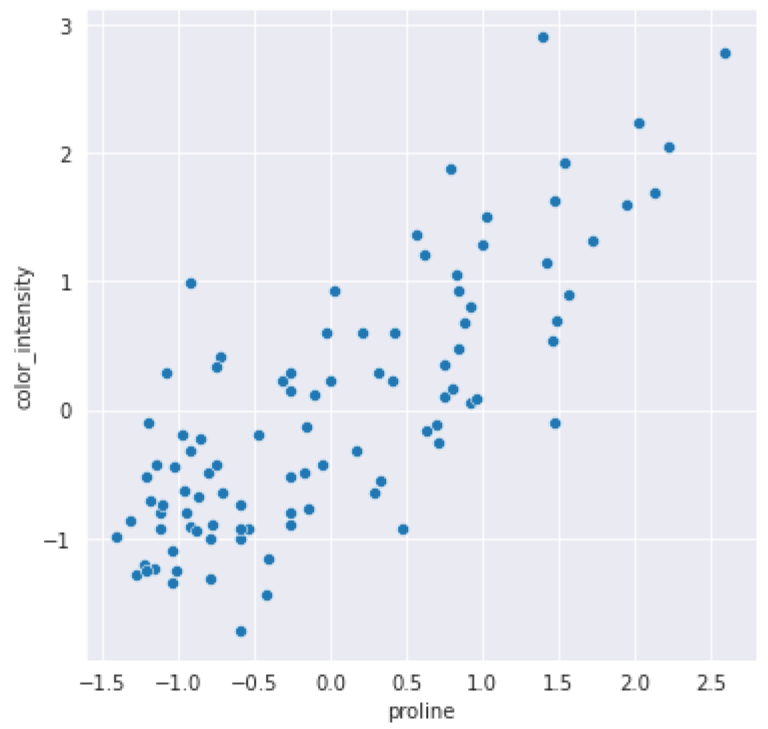
- Unsupervised Learning method (ignores label)
- Idea:
    - Directions of high variance in the data contain important information
    - Colinear features can be combined
    - Find directions of maximum variance
    - Project onto subspace with same or fewer dimensions

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

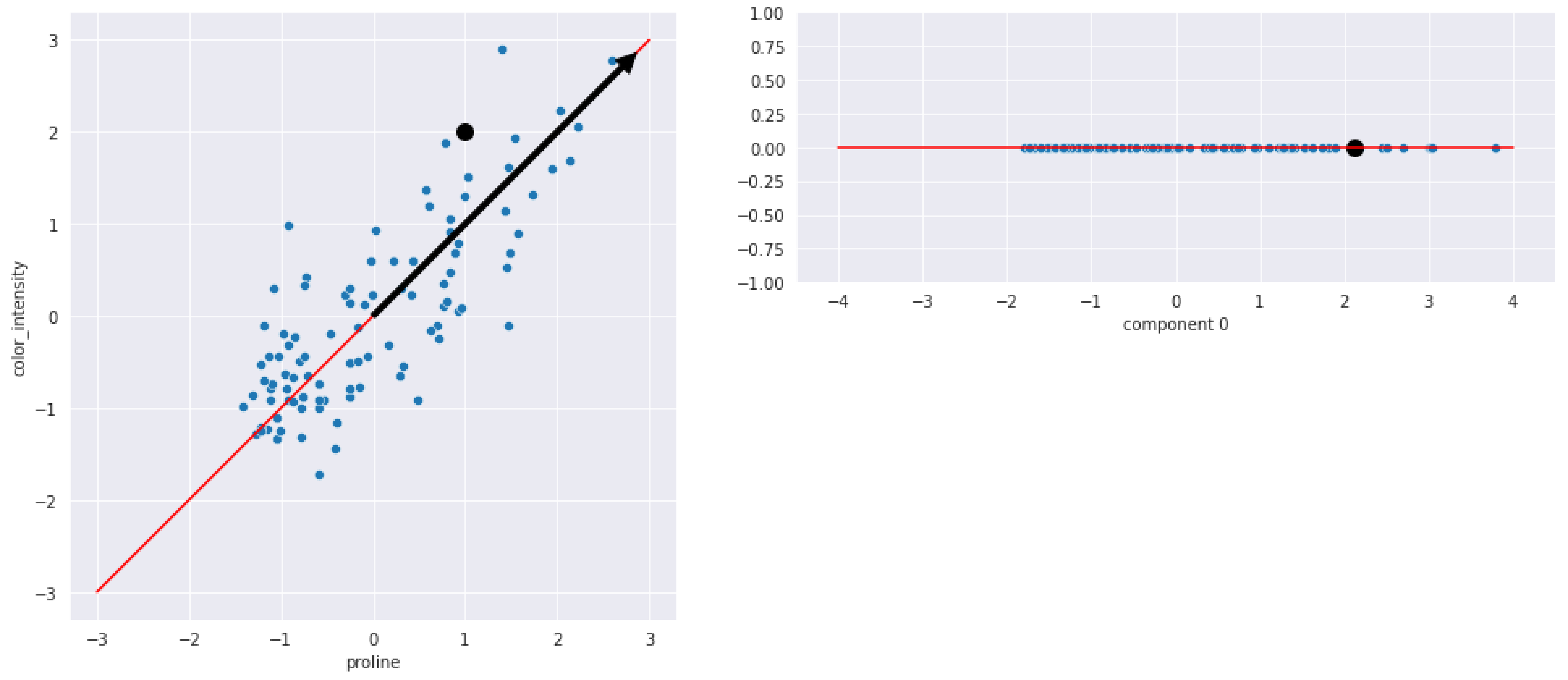
PCA Example

In [26]:
```
fig,ax = plt.subplots(1,1,figsize=(6,6))
sns.scatterplot(x='proline',y='color_intensity',data=X_train,ax=ax);
```



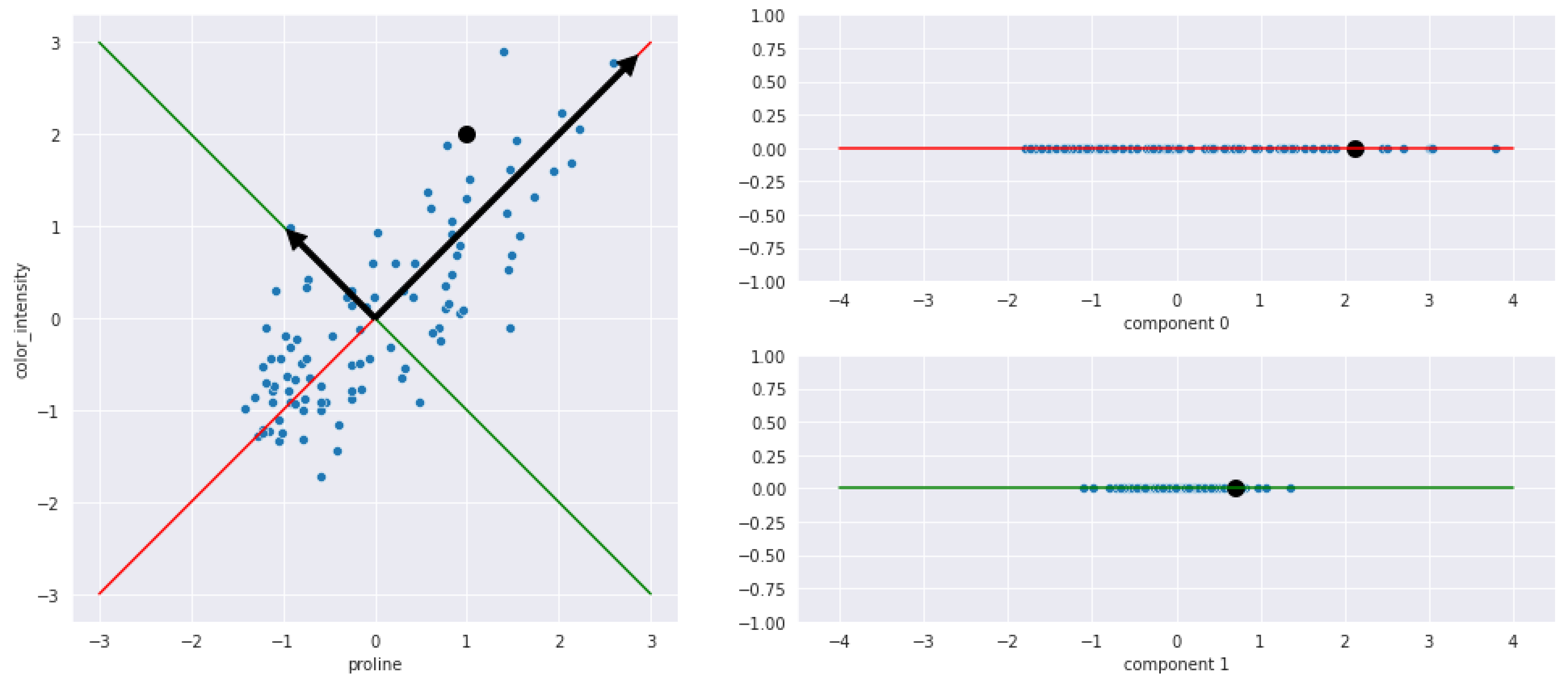
PCA Example Cont.

```
In [28]: plot_pca(X_train[['proline','color_intensity']],pca,num_components=1)
         plt.tight_layout()
```



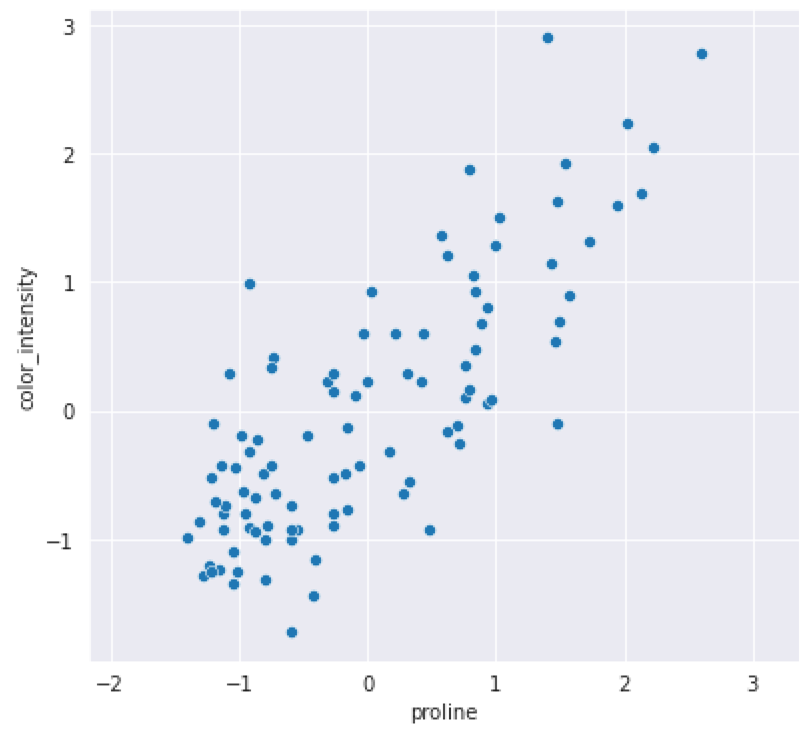
PCA Example Cont.

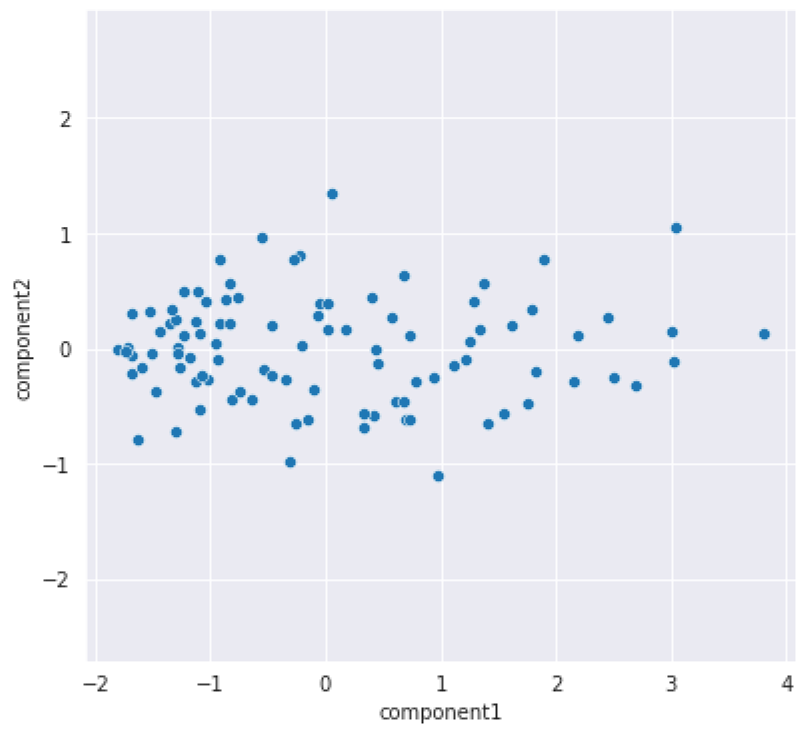
In [29]:
```
plot_pca(X_train[['proline','color_intensity']],pca,num_components=2)
plt.tight_layout()
```



PCA in sklearn

In [30]:
```
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?

```
In [31]: pca.explained_variance_ratio_

Out[31]: array([0.89808764, 0.10191236])
```

PCA: Principle Components

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

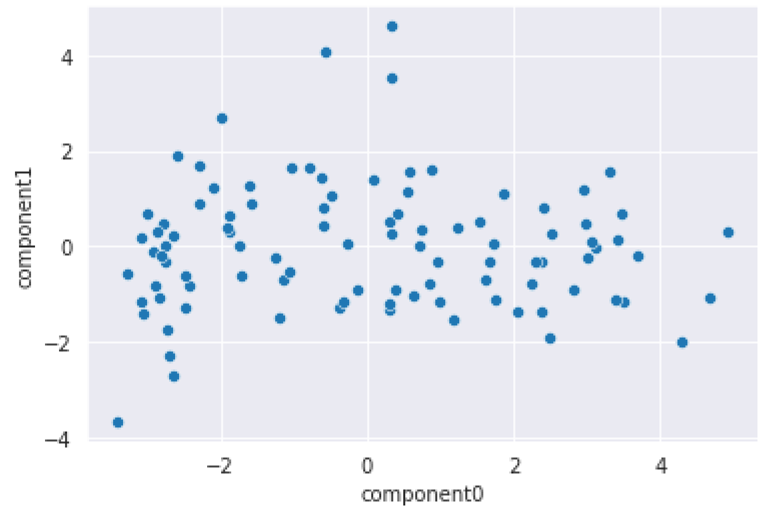
```
In [32]: pca.components_[0]

Out[32]: array([0.70710678, 0.70710678])
```

- And the second?

```
In [33]: pca.components_[1]

Out[33]: array([-0.70710678,  0.70710678])
```

Dimensionality Reduction with PCA

In [34]:
```
pca_2d = PCA(n_components=2)
X_2d = pca_2d.fit_transform(X_train,y_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 [35]:
```
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
```

PCA and Image Recognition

- Generally, 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!

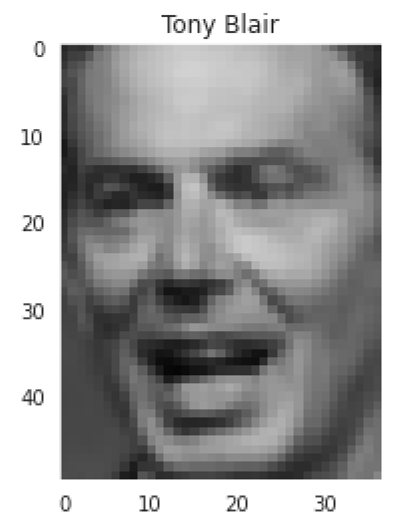
- Image classification using PCA?
  - Example based on Faces recognition example using eigenfaces and SVMs

Example Dataset: LFW

Labeled Faces in the Wild

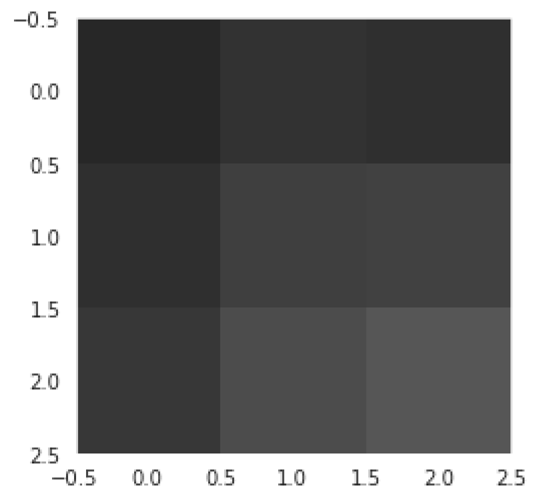
In [36]:
```
from sklearn.datasets import fetch_lfw_people

lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)
```

In [37]:
```
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

In [38]:
```
# first 3x3 set of pixels
plt.imshow(lfw_people.images[1][:3,:3],cmap=plt.cm.gray,vmin=0, vmax=255);
```



In [39]:
```
lfw_people.images[1][:3,:3]
```

Out[39]:
```
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?

```
In [40]: lfw_people.images[1].shape

Out[40]: (50, 37)

In [41]: x = lfw_people.images[1].reshape(1,-1)
         x

Out[41]: array([[ 39.666668,  50.333332,  47.       , ..., 117.666664, 115.       ,
                 133.66667 ]], dtype=float32)

In [42]: x.shape

Out[42]: (1, 1850)
```

What information do we lose when we do this?

Create a Dataset

```
In [43]: # 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,
                                                                                     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
```

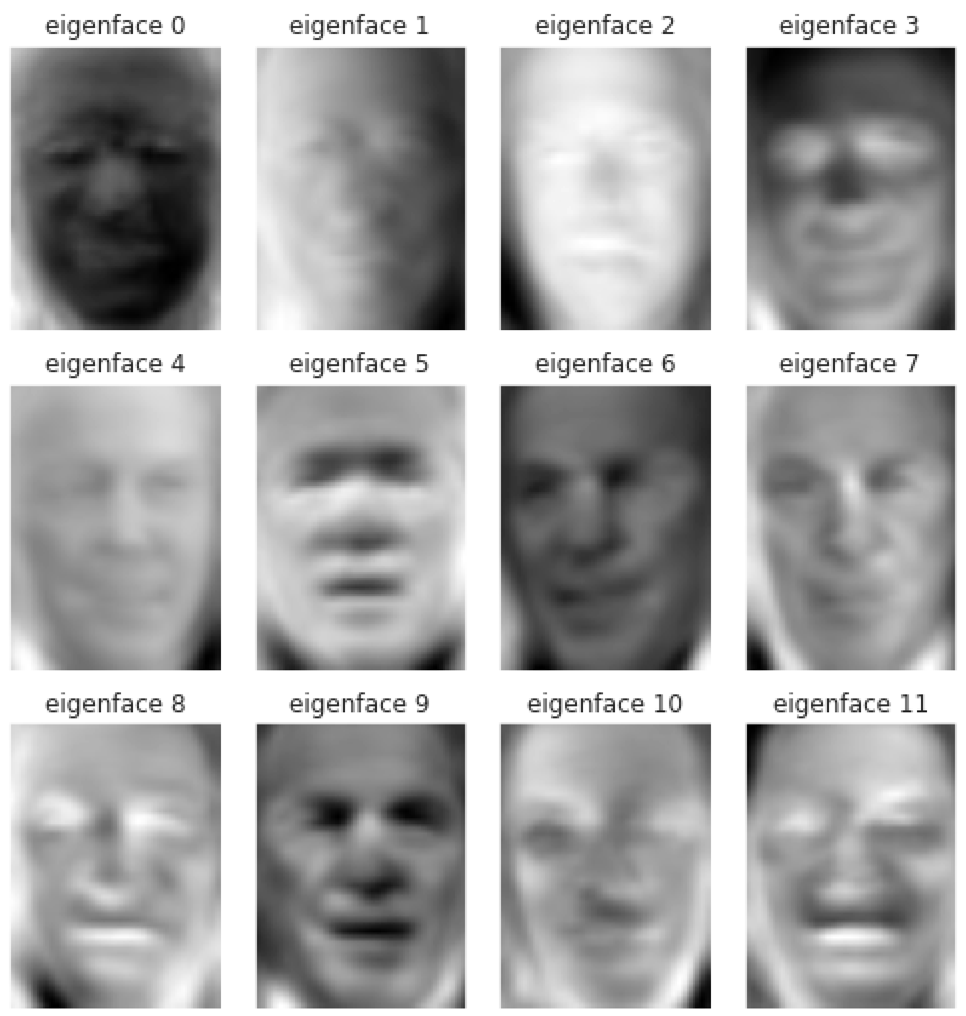
Compute PCA and Transform

```
In [44]: # 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)
```

Eigenfaces

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

In [46]:
```
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

In [47]:
```
%%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 607 ms, sys: 122 ms, total: 729 ms
Wall time: 6.85 s
```

In [48]:
```
print(f"best_params : {clf_faces.best_params_}")
print(f"best_score  : {clf_faces.best_score_:0.2f}")
```

```
best_params : {'C': 1000.0, 'gamma': 0.001}
best_score  : 0.78
```

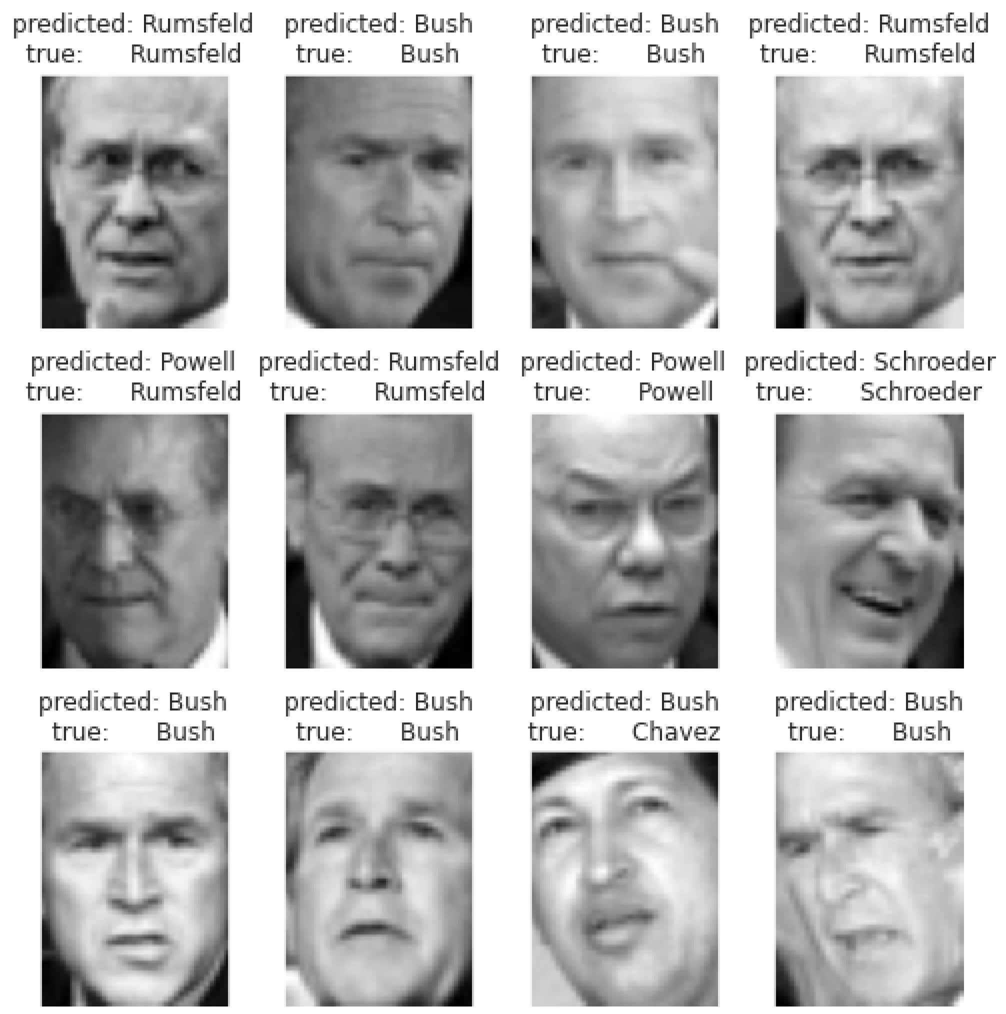
Evaluate on the test set

```
In [49]: 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       0.70      0.47      0.56        15
     Colin Powell       0.74      0.84      0.79        55
  Donald Rumsfeld       0.91      0.70      0.79        43
    George W Bush       0.87      0.93      0.90       135
Gerhard Schroeder       0.75      0.88      0.81        24
      Hugo Chavez       0.83      0.59      0.69        17
       Tony Blair       0.82      0.82      0.82        33

         accuracy                           0.83       322
        macro avg       0.80      0.74      0.76       322
     weighted avg       0.83      0.83      0.82       322
```

Prediction Examples

```
In [50]: 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()
```

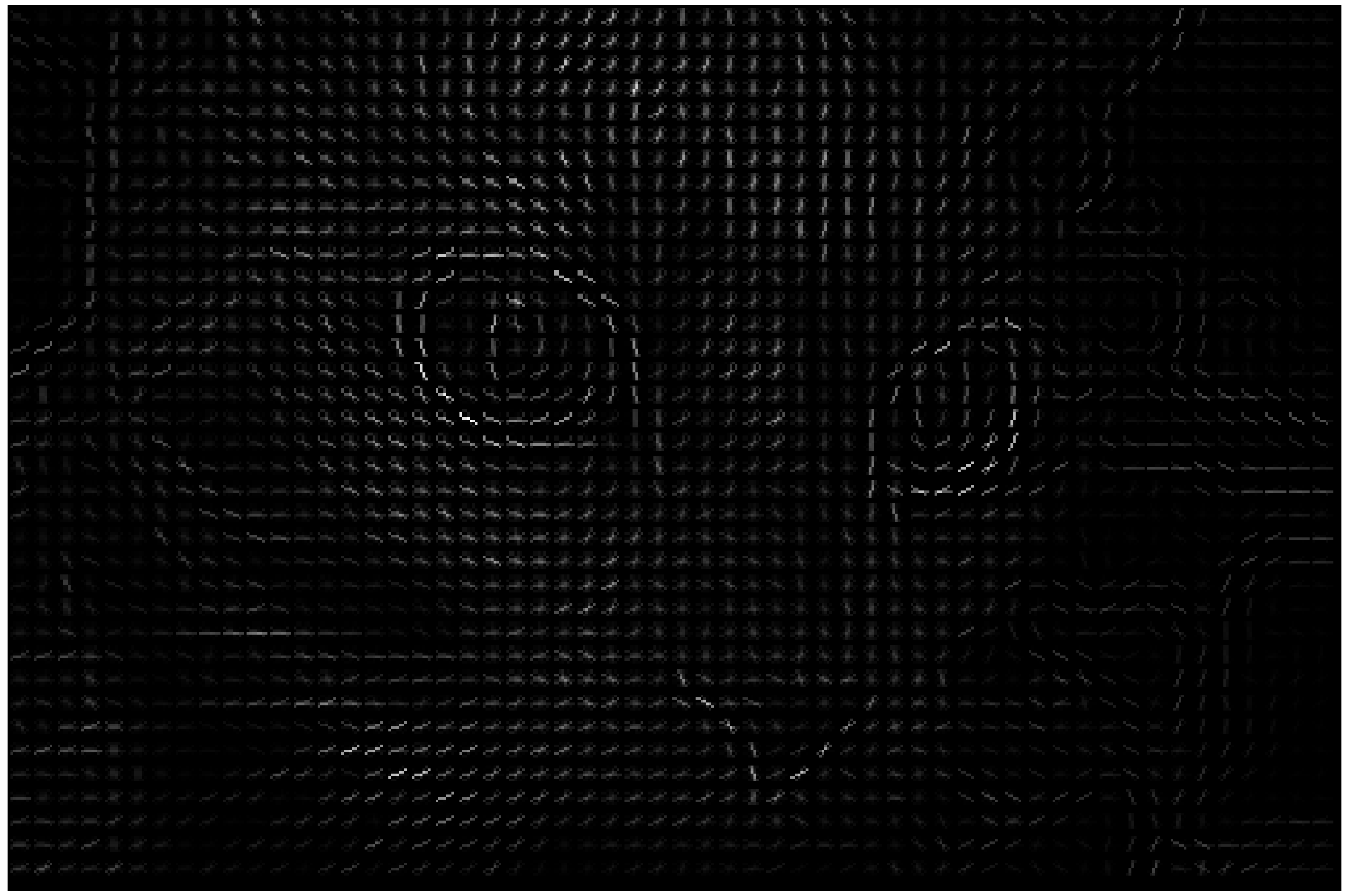


Performance without PCA

```
%%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

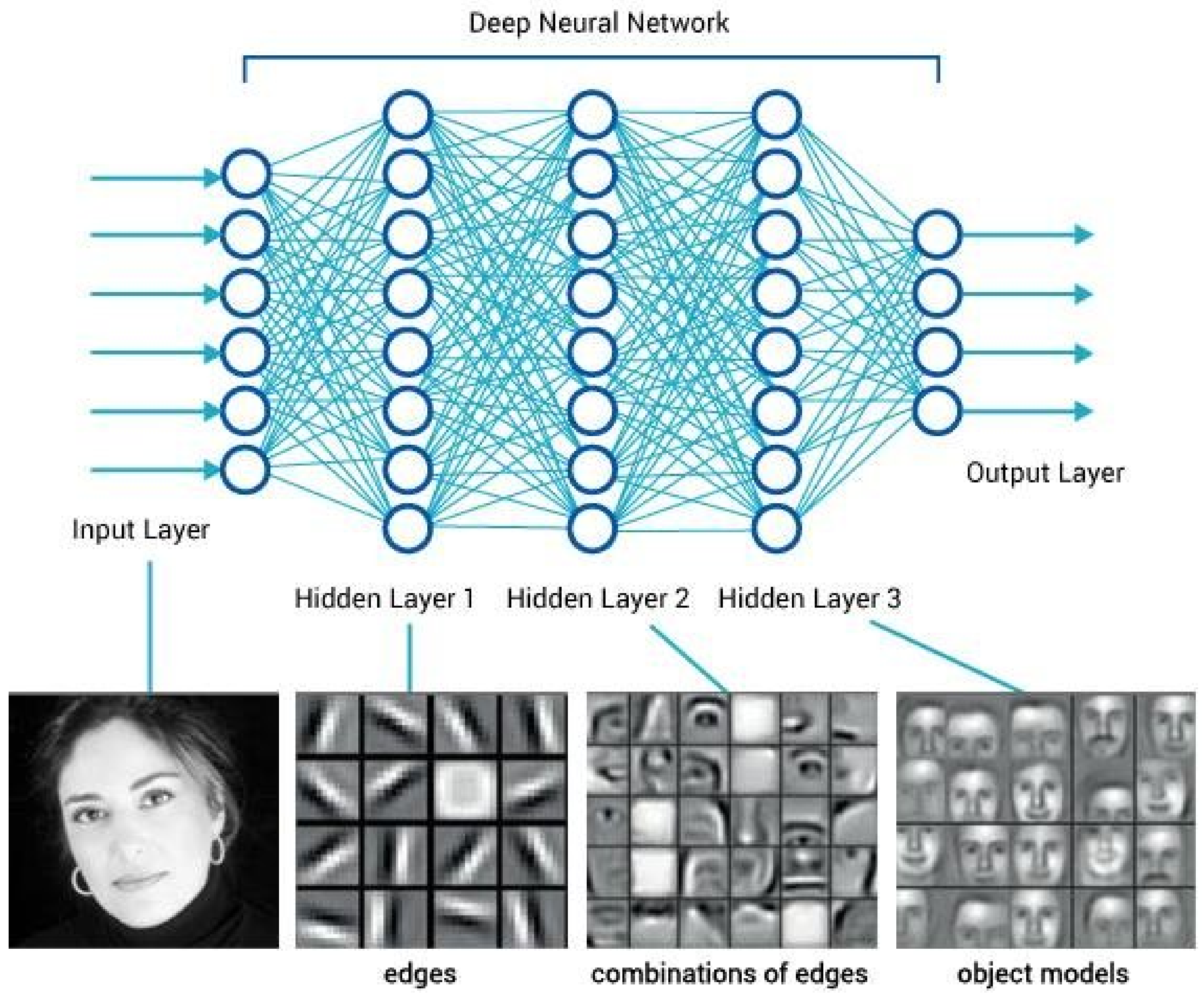
- With Feature Engineering and general models
  - ex: Histogram of Oriented Gradients or HOG (See PDSH Chap 5)
  - many more (See scikit-image)



From PDSH

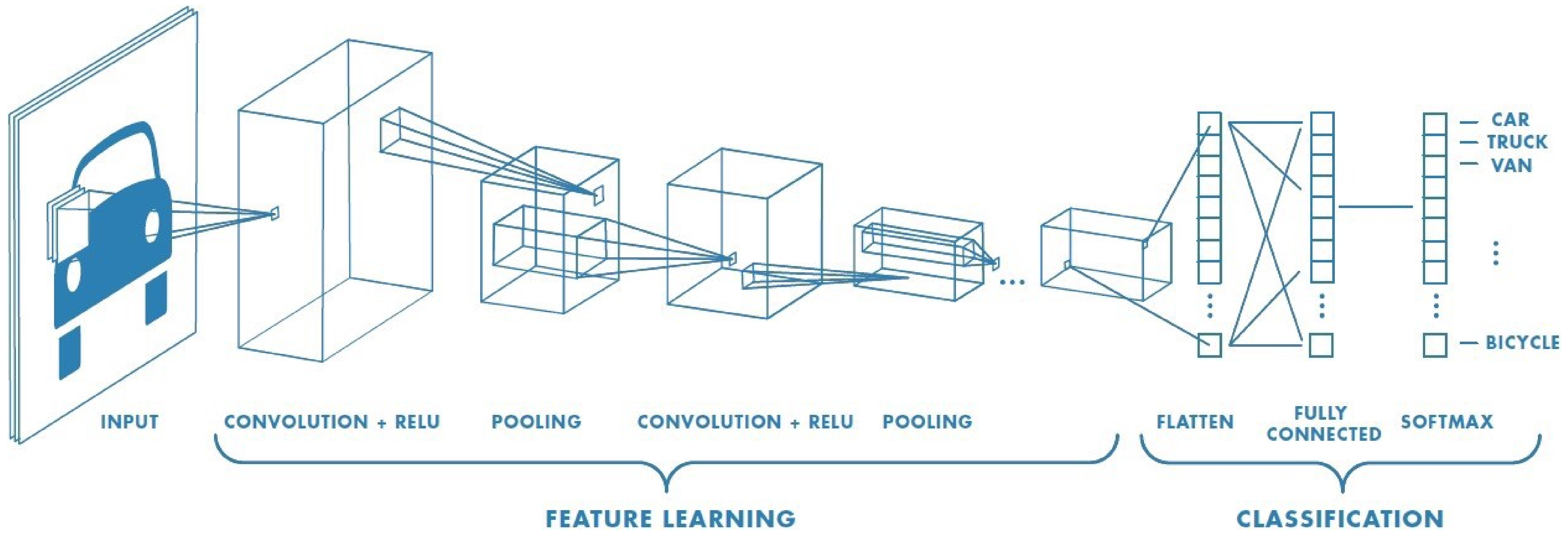
Other Image Recognition Methods: Deep Neural Networks

- 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?