Lecture 18 Part 2 - PCA Implementations & Applications

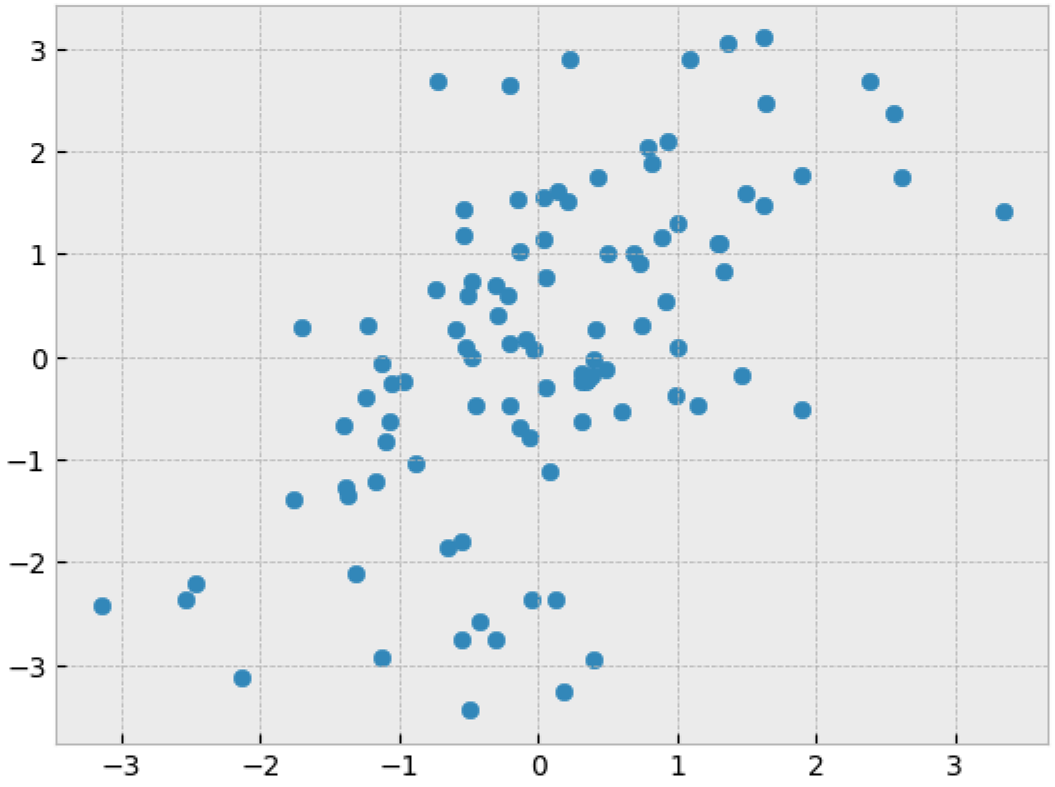
In [5]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
plt.style.use('bmh')
```

In [6]:
```
# Helper functions

def plotvec(*argv):
    colors=['k','b','r','g','c','m']
    xmin=0
    xmax=-1000000
    ymin=0
    ymax=-1000000
    origin=[0,0]
#     plt.figure()
    for e in enumerate(argv):
        i=e[0]
        arg=e[1]
        plt.quiver(*origin,*arg,angles='xy',scale_units='xy',scale=1,
                   color=colors[i%len(colors)])
        xmin=min(xmin,arg[0])
        xmax=max(xmax,arg[0])
        ymin=min(ymin,arg[1])
        ymax=max(ymax,arg[1])
#     plt.xlim(min(-1, xmin-1), max(1,xmax+1))
#     plt.ylim(min(-1,ymin-1),max(1,ymax+1))

def plot_contours(K,X=None, R=None):
    '''This function plots the contours of a Bivariate Gaussian RV with
    mean [0,0] and covariance K'''

    x = np.linspace(-4, 4, 100)
    y = np.linspace(-4, 4, 100)
    xm, ym = np.meshgrid(x, np.flip(y))
    if X is None:
        X = np.dstack([xm,ym])
    if R is not None:
        X = X@R

    G = stats.multivariate_normal.pdf(X,mean=[0,0],cov=K)

    plt.figure(figsize=(6,6))
    plt.contour(xm,ym,G, extent=[-3,3,-3,3],cmap='viridis');

def makerot(theta):
    '''This function creates a 2x2 rotation
    matrix for a given angle (theta) in degrees'''

    theta=np.radians(theta)

    R = np.array([[np.cos(theta), -np.sin(theta)],
                  [np.sin(theta), np.cos(theta)]])

    return R
```

In [7]:
```
import scipy.stats as stats

data = stats.multivariate_normal([0,0],[[1,0.8],[0.8,2]]).rvs(size=100)

data.shape
```

Out[7]:
```
(100, 2)
```

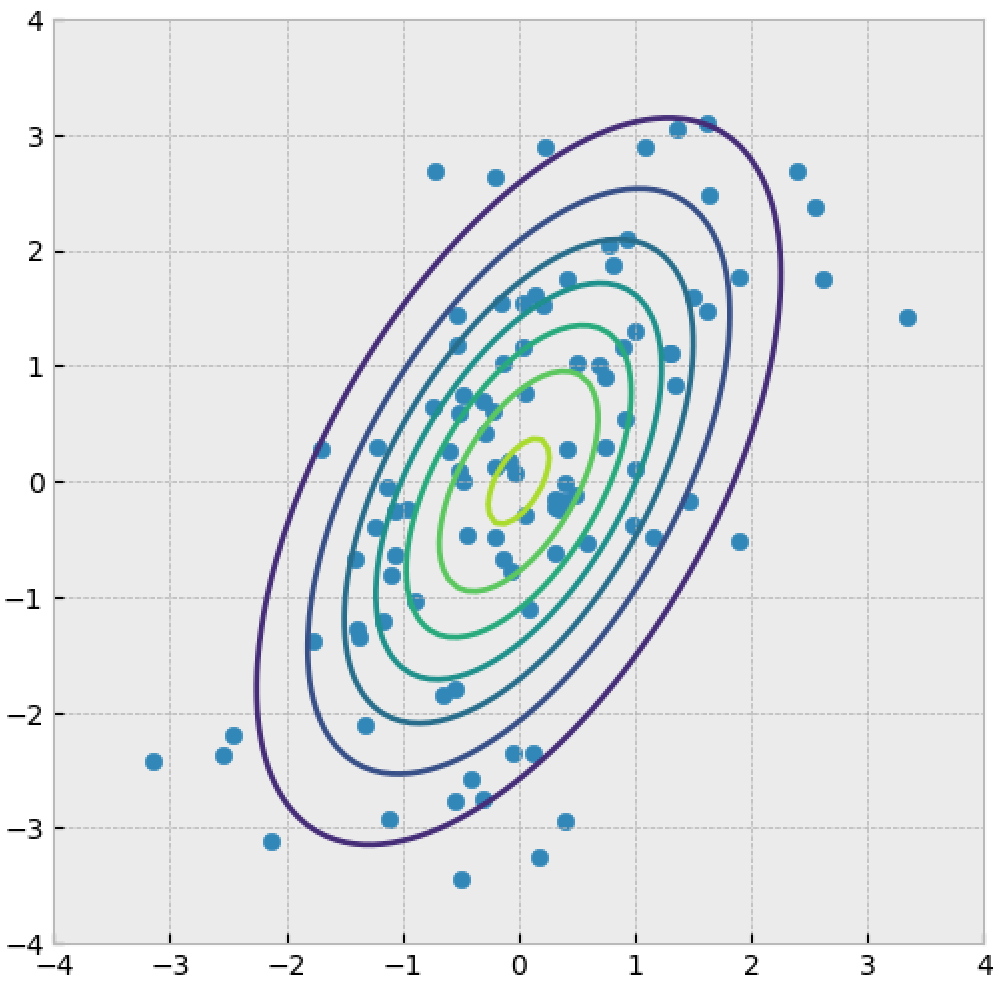
In [8]:
```
plt.scatter(data[:,0],data[:,1]);
```



In [9]:
```
# Covariance matrix of input matrix
K = np.cov(data.T)

K
```

Out[9]:
```
array([[1.28769712, 1.02672147],
       [1.02672147, 2.50736883]])
```

In [10]:
```
plot_contours(K)
plt.scatter(data[:,0],data[:,1]);
```



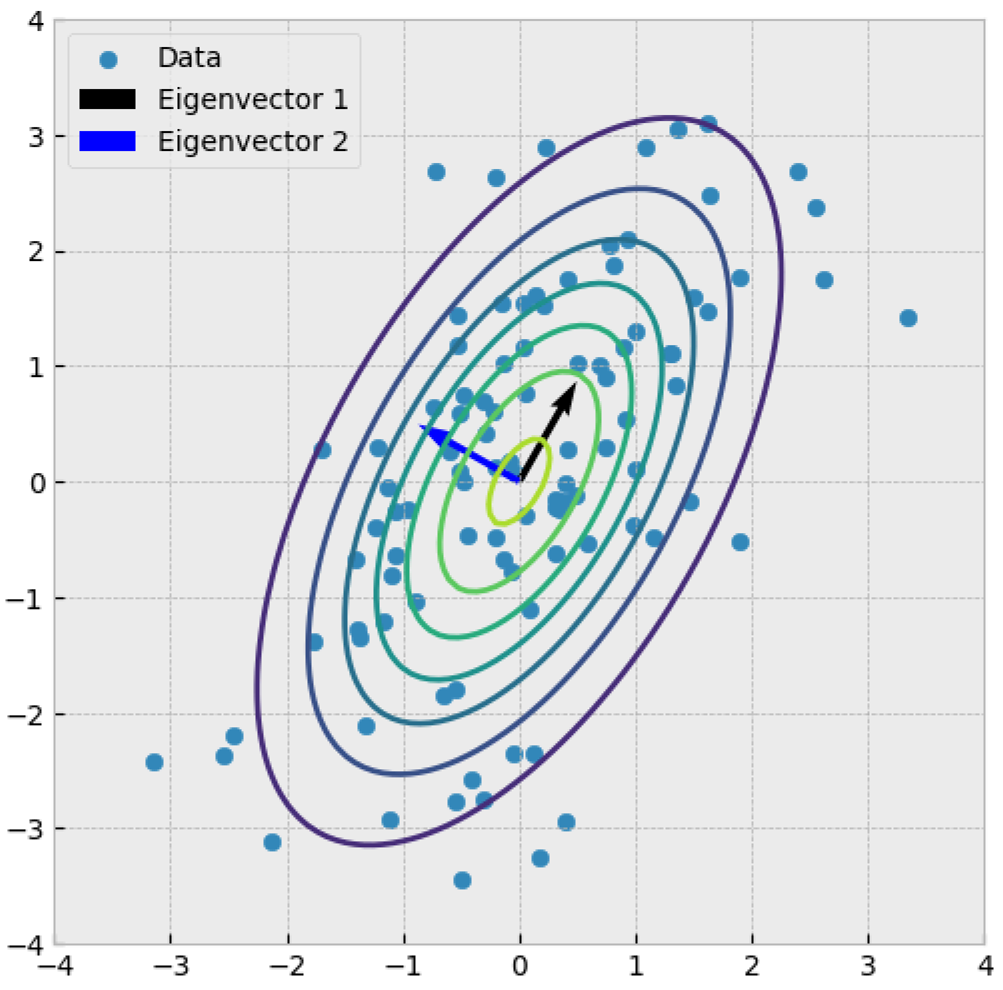
In [11]:
```
# Eigendecomposition
L, V = np.linalg.eigh(K)

L, V
```

Out[11]:
```
(array([0.70335679, 3.09170915]),
 array([[-0.86910153,  0.49463373],
        [ 0.49463373,  0.86910153]]))
```

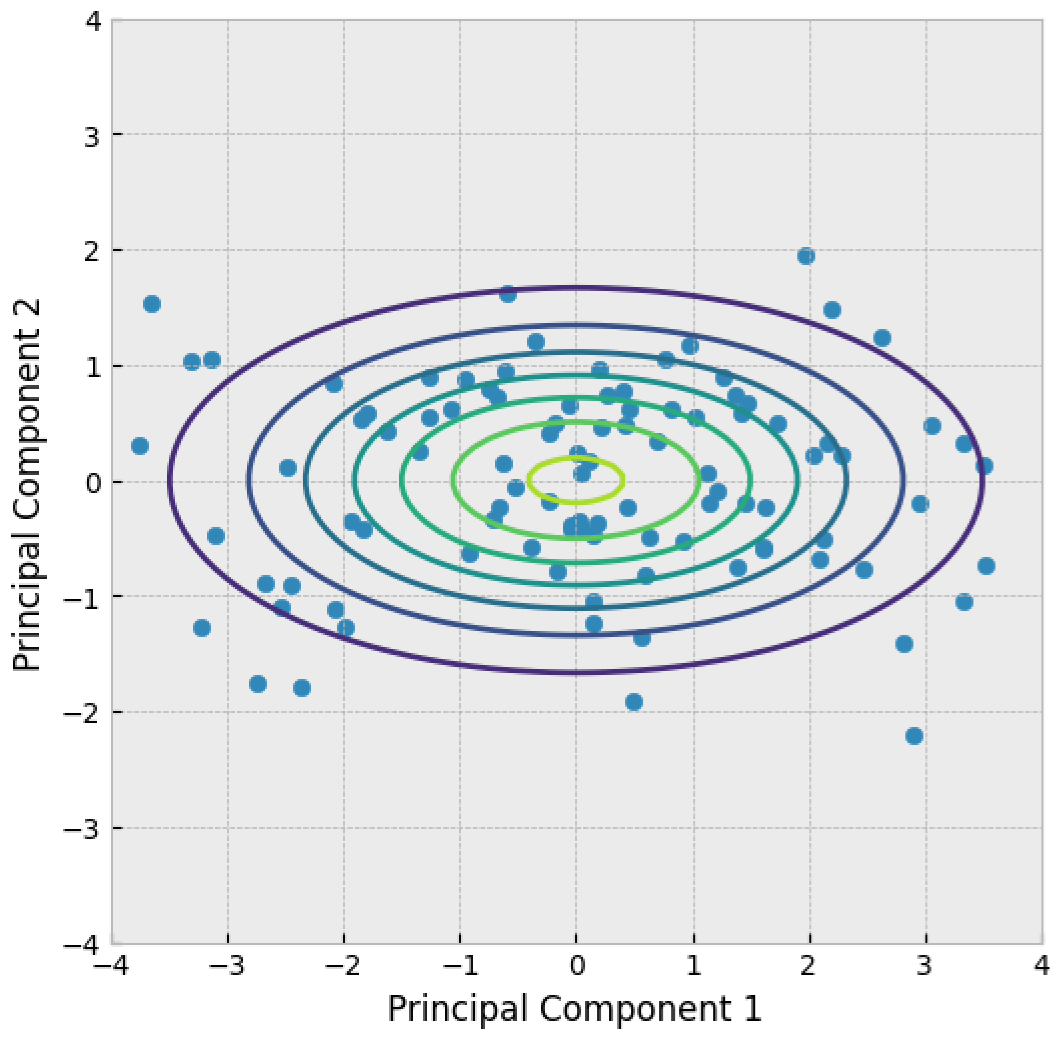
In [12]:
```
# Sort eigenvalues and eigenvectors in decreasing order of eigenvalues

L=L[::-1]

V=V[:,::-1]

L, V
```

Out[12]:
```
(array([3.09170915, 0.70335679]),
 array([[ 0.49463373, -0.86910153],
        [ 0.86910153,  0.49463373]]))
```

In [13]:
```
plot_contours(K)
plt.scatter(data[:,0],data[:,1])
plotvec(V[:,0], V[:,1])
plt.legend(['Data','Eigenvector 1', 'Eigenvector 2']);
```



```
In [14]: # Apply PCA to preserve dimensions == rotating the data
         rotated =  V.T@data.T

         rotated.shape

Out[14]: (2, 100)

In [15]: # Check the covariance of PCA transformation
         K2 = np.cov(rotated)

         np.round(K2,7)

Out[15]: array([[3.0917092, 0.       ],
                [0.       , 0.7033568]])

In [16]: plot_contours(K2)
         plt.scatter(rotated[0,:],rotated[1,:])
         plt.xlabel('Principal Component 1')
         plt.ylabel('Principal Component 2');
```



In [17]:
```
# standard unit vector
e1=np.array([[1],[0]])

angle = np.degrees(np.arccos((e1.T@V[:,0])/(np.linalg.norm(e1)*np.linalg.norm(V[:,0

angle
```

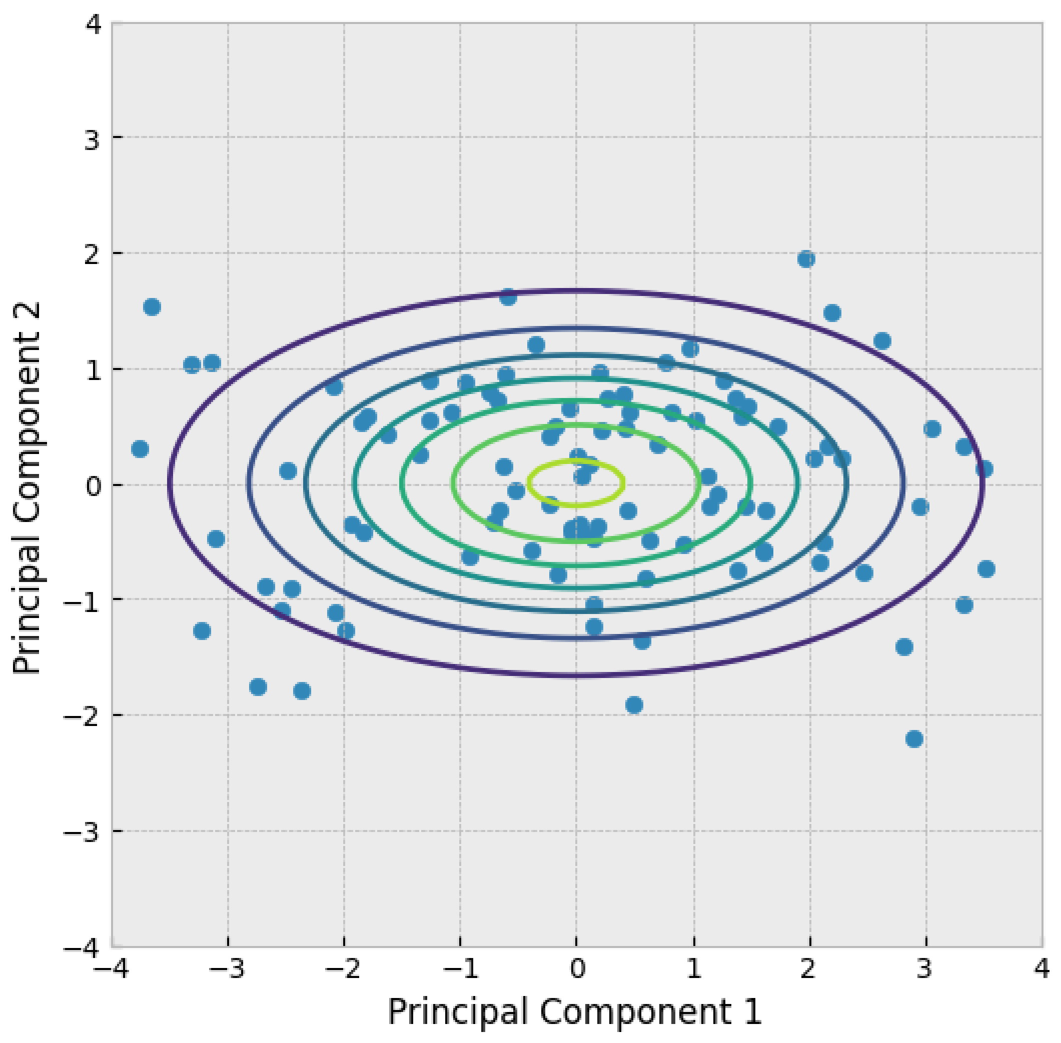
Out[17]:
```
60.35439904480175
```

In [18]:
```
# Apply manual rotation

rotated2 = makerot(-angle)@data.T
```

In [19]:
```
K3 = np.cov(rotated2)

np.round(K3,7)
```

Out[19]:
```
array([[3.0917092, 0.       ],
       [0.       , 0.7033568]])
```

In [20]:
```
plot_contours(K3)
plt.scatter(rotated2[0,:],rotated2[1,:])
plt.xlabel('Principal Component 1')
plt.ylabel('Principal Component 2');
```



In [21]:
```
import pandas as pd
from scipy import stats
import numpy as np
import numpy.random as npr
import matplotlib.pyplot as plt
%matplotlib inline
plt.style.use('bmh')
plt.rcParams['axes.grid'] = False

from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler, MinMaxScaler
from sklearn.pipeline import Pipeline
```

In [22]:
```
def myPCA(X, m, display=1):
    '''This function implements PCA. The data matrix X is DxN matrix,
    where D is the dimension and N the number of points'''

    D, N = X.shape
    # Demean the Data
    data = X

    # Covariance of the input data X
    cov_mat = np.cov(data) # is data were to be NxD, np.cov(data.T)

    # Find eigenvectors and eigenvalues
    eigen_vals, eigen_vecs = np.linalg.eigh(cov_mat)
    # eigendecomposition for Hermitian matrices (positive-definite matrices)-which

    # Sort eigenvectors by magnitude of eigenvalues
    L = eigen_vals[::-1]
    U = eigen_vecs[:,::-1]

    # Linear transformation
    A = U[:,:m]

    #compute explained variance and plot
    cuml_var_exp=0
    total = sum(L)
    var_explained = [(i/total) for i in L]
    cuml_var_exp = np.cumsum(var_explained)
    if display:
        plt.bar(range(1,D+1), var_explained, alpha=0.5, align='center', label='indi
        plt.step(range(1,D+1), cuml_var_exp, alpha=0.5, where='mid', label='cumulat
        plt.ylabel('Explained variance ratio')
        plt.xlabel('Principal components')
        plt.legend(loc='best');
    return A, var_explained
```

Coming back to the wine dataset:

In [23]:
```
df_wine = pd.read_csv('https://archive.ics.uci.edu/ml/machine-learning-databases/wi

df_wine.columns = ['Class label', 'Alcohol',
                   'Malic acid', 'Ash',
                   'Alcalinity of ash', 'Magnesium',
                   'Total phenols', 'Flavanoids',
                   'Nonflavanoid phenols',
                   'Proanthocyanins',
                   'Color intensity', 'Hue',
                   'OD280/OD315 of diluted wines',
                   'Proline']


df_wine
```

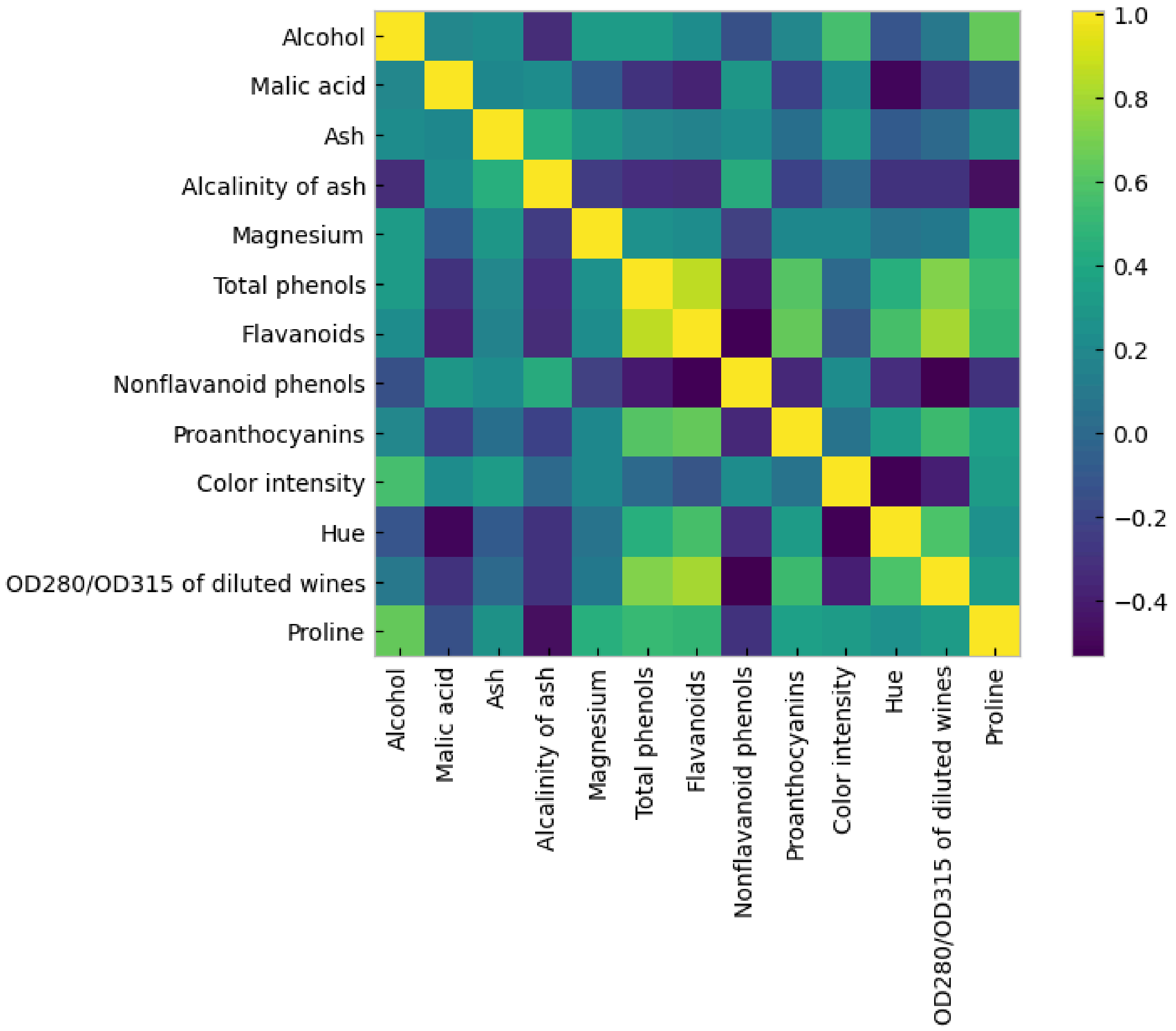
Out[23]:

	Class label	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoi phenol
0	1	14.23	1.71	2.43	15.6	127	2.80	3.06	0.2
1	1	13.20	1.78	2.14	11.2	100	2.65	2.76	0.2
2	1	13.16	2.36	2.67	18.6	101	2.80	3.24	0.3
3	1	14.37	1.95	2.50	16.8	113	3.85	3.49	0.2
4	1	13.24	2.59	2.87	21.0	118	2.80	2.69	0.3
...	...	...	...	...	...	...	...	...	.
173	3	13.71	5.65	2.45	20.5	95	1.68	0.61	0.5
174	3	13.40	3.91	2.48	23.0	102	1.80	0.75	0.4
175	3	13.27	4.28	2.26	20.0	120	1.59	0.69	0.4
176	3	13.17	2.59	2.37	20.0	120	1.65	0.68	0.5
177	3	14.13	4.10	2.74	24.5	96	2.05	0.76	0.5

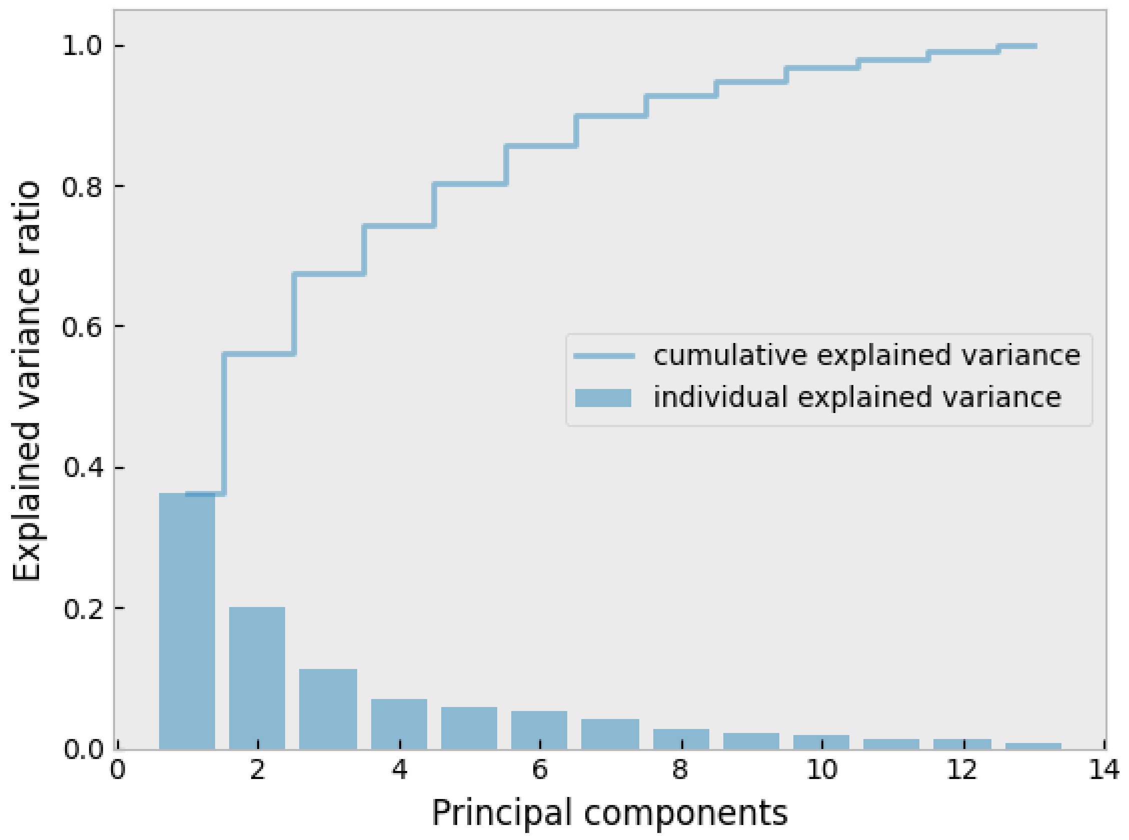
178 rows × 14 columns

In [24]:
```
t = df_wine['Class label'].values
X = df_wine.drop(['Class label'], axis=1).values

X_train, X_test, t_train, t_test = train_test_split(X, t,
                                                    test_size=0.3,
                                                    stratify=t)

scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

In [25]:
```
cov_train = np.cov(X_train.T)

plt.figure(figsize=(8,5))
plt.imshow(cov_train)
plt.colorbar()
plt.xticks(range(13),df_wine.columns[1:],rotation=90)
plt.yticks(range(13),df_wine.columns[1:]);
```



```
In [26]: X_train.shape

Out[26]: (124, 13)

In [27]: A,var_explained = myPCA(X_train.T, 13)

         A.shape

Out[27]: (13, 13)
```



The resulting plot indicates that the first principal component alone accounts for 40 percent of the variance. Also, we can see that the first two principal components combined explain almost 60 percent of the variance in the data.

Although the explained variance plot reminds us of the feature importance, we shall remind ourselves that PCA is an unsupervised method, which means that information about the class labels is ignored.

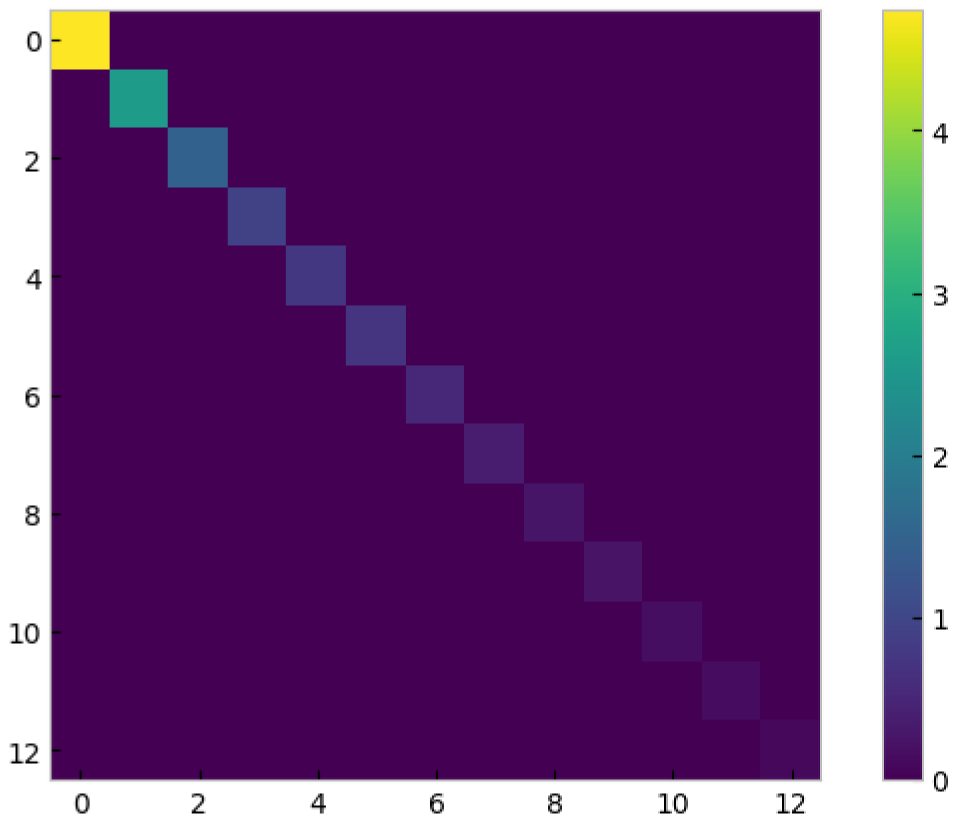
```
In [28]: np.where(np.cumsum(var_explained)>=0.9)
```

```
Out[28]: (array([ 7,  8,  9, 10, 11, 12], dtype=int64),)
```

```
In [29]: X_train_pca = A.T@X_train.T

         print(X_train.shape, X_train_pca.shape)
```

```
(124, 13) (13, 124)
```

```
In [30]: cov_mat = np.cov(X_train_pca)

         plt.figure(figsize=(8,5))
         plt.imshow(cov_mat)
         plt.colorbar();
```



PCA with `scikit-learn`

```
In [31]: from sklearn.decomposition import PCA
```

```
In [32]: PCA?
```

```
Init signature:
PCA(
    n_components=None,
    *,
    copy=True,
    whiten=False,
    svd_solver='auto',
    tol=0.0,
    iterated_power='auto',
    n_oversamples=10,
    power_iteration_normalizer='auto',
    random_state=None,
)
Docstring:
Principal component analysis (PCA).

Linear dimensionality reduction using Singular Value Decomposition of the
data to project it to a lower dimensional space. The input data is centered
but not scaled for each feature before applying the SVD.

It uses the LAPACK implementation of the full SVD or a randomized truncated
SVD by the method of Halko et al. 2009, depending on the shape of the input
data and the number of components to extract.

It can also use the scipy.sparse.linalg ARPACK implementation of the
truncated SVD.

Notice that this class does not support sparse input. See
:class:`TruncatedSVD` for an alternative with sparse data.

For a usage example, see
:ref:`sphx_glr_auto_examples_decomposition_plot_pca_iris.py`

Read more in the :ref:`User Guide <PCA>`.

Parameters
----------
n_components : int, float or 'mle', default=None
    Number of components to keep.
    if n_components is not set all components are kept::

        n_components == min(n_samples, n_features)

    If ``n_components == 'mle'`` and ``svd_solver == 'full'``, Minka's
    MLE is used to guess the dimension. Use of ``n_components == 'mle'``
    will interpret ``svd_solver == 'auto'`` as ``svd_solver == 'full'``.

    If ``0 < n_components < 1`` and ``svd_solver == 'full'``, select the
    number of components such that the amount of variance that needs to be
    explained is greater than the percentage specified by n_components.

    If ``svd_solver == 'arpack'``, the number of components must be
    strictly less than the minimum of n_features and n_samples.

    Hence, the None case results in::
        n_components == min(n_samples, n_features) - 1

copy : bool, default=True
    If False, data passed to fit are overwritten and running
    fit(X).transform(X) will not yield the expected results,
    use fit_transform(X) instead.

whiten : bool, default=False
    When True (False by default) the `components_` vectors are multiplied
    by the square root of n_samples and then divided by the singular values
    to ensure uncorrelated outputs with unit component-wise variances.

    Whitening will remove some information from the transformed signal
    (the relative variance scales of the components) but can sometime
    improve the predictive accuracy of the downstream estimators by
    making their data respect some hard-wired assumptions.

svd_solver : {'auto', 'full', 'arpack', 'randomized'}, default='auto'
    If auto :
        The solver is selected by a default policy based on `X.shape` and
        `n_components`: if the input data is larger than 500x500 and the
        number of components to extract is lower than 80% of the smallest
        dimension of the data, then the more efficient 'randomized'
        method is enabled. Otherwise the exact full SVD is computed and
        optionally truncated afterwards.
    If full :
        run exact full SVD calling the standard LAPACK solver via
        `scipy.linalg.svd` and select the components by postprocessing
    If arpack :
        run SVD truncated to n_components calling ARPACK solver via
        `scipy.sparse.linalg.svds`. It requires strictly
        0 < n_components < min(X.shape)
    If randomized :
        run randomized SVD by the method of Halko et al.

    .. versionadded:: 0.18.0

tol : float, default=0.0
    Tolerance for singular values computed by svd_solver == 'arpack'.
    Must be of range [0.0, infinity).

    .. versionadded:: 0.18.0

iterated_power : int or 'auto', default='auto'
    Number of iterations for the power method computed by
    svd_solver == 'randomized'.
    Must be of range [0, infinity).

    .. versionadded:: 0.18.0

n_oversamples : int, default=10
    This parameter is only relevant when `svd_solver="randomized"`.
    It corresponds to the additional number of random vectors to sample the
    range of `X` so as to ensure proper conditioning. See
    :func:`~sklearn.utils.extmath.randomized_svd` for more details.
```

```
        .. versionadded:: 1.1

    power_iteration_normalizer : {'auto', 'QR', 'LU', 'none'}, default='auto'
        Power iteration normalizer for randomized SVD solver.
        Not used by ARPACK. See :func:`~sklearn.utils.extmath.randomized_svd`
        for more details.

        .. versionadded:: 1.1

    random_state : int, RandomState instance or None, default=None
        Used when the 'arpack' or 'randomized' solvers are used. Pass an int
        for reproducible results across multiple function calls.
        See :term:`Glossary <random_state>`.

        .. versionadded:: 0.18.0

    Attributes
    ----------
    components_ : ndarray of shape (n_components, n_features)
        Principal axes in feature space, representing the directions of
        maximum variance in the data. Equivalently, the right singular
        vectors of the centered input data, parallel to its eigenvectors.
        The components are sorted by decreasing ``explained_variance_``.

    explained_variance_ : ndarray of shape (n_components,)
        The amount of variance explained by each of the selected components.
        The variance estimation uses `n_samples - 1` degrees of freedom.

        Equal to n_components largest eigenvalues
        of the covariance matrix of X.

        .. versionadded:: 0.18

    explained_variance_ratio_ : ndarray of shape (n_components,)
        Percentage of variance explained by each of the selected components.

        If ``n_components`` is not set then all components are stored and the
        sum of the ratios is equal to 1.0.

    singular_values_ : ndarray of shape (n_components,)
        The singular values corresponding to each of the selected components.
        The singular values are equal to the 2-norms of the ``n_components``
        variables in the lower-dimensional space.

        .. versionadded:: 0.19

    mean_ : ndarray of shape (n_features,)
        Per-feature empirical mean, estimated from the training set.

        Equal to `X.mean(axis=0)`.

    n_components_ : int
        The estimated number of components. When n_components is set
        to 'mle' or a number between 0 and 1 (with svd_solver == 'full') this
        number is estimated from input data. Otherwise it equals the parameter
        n_components, or the lesser value of n_features and n_samples
        if n_components is None.

    n_samples_ : int
        Number of samples in the training data.

    noise_variance_ : float
        The estimated noise covariance following the Probabilistic PCA model
        from Tipping and Bishop 1999. See "Pattern Recognition and
        Machine Learning" by C. Bishop, 12.2.1 p. 574 or
        http://www.miketipping.com/papers/met-mppca.pdf. It is required to
        compute the estimated data covariance and score samples.

        Equal to the average of (min(n_features, n_samples) - n_components)
        smallest eigenvalues of the covariance matrix of X.

    n_features_in_ : int
        Number of features seen during :term:`fit`.

        .. versionadded:: 0.24

    feature_names_in_ : ndarray of shape (`n_features_in_`,)
        Names of features seen during :term:`fit`. Defined only when `X`
        has feature names that are all strings.

        .. versionadded:: 1.0

    See Also
    --------
    KernelPCA : Kernel Principal Component Analysis.
    SparsePCA : Sparse Principal Component Analysis.
    TruncatedSVD : Dimensionality reduction using truncated SVD.
    IncrementalPCA : Incremental Principal Component Analysis.

    References
    ----------
    For n_components == 'mle', this class uses the method from:
    `Minka, T. P.. "Automatic choice of dimensionality for PCA".
    In NIPS, pp. 598-604 <https://tminka.github.io/papers/pca/minka-pca.pdf>`_

    Implements the probabilistic PCA model from:
    `Tipping, M. E., and Bishop, C. M. (1999). "Probabilistic principal
    component analysis". Journal of the Royal Statistical Society:
    Series B (Statistical Methodology), 61(3), 611-622.
    <http://www.miketipping.com/papers/met-mppca.pdf>`_
    via the score and score_samples methods.

    For svd_solver == 'arpack', refer to `scipy.sparse.linalg.svds`.

    For svd_solver == 'randomized', see:
    :doi:`Halko, N., Martinsson, P. G., and Tropp, J. A. (2011).
    "Finding structure with randomness: Probabilistic algorithms for
    constructing approximate matrix decompositions".
    SIAM review, 53(2), 217-288.
    <10.1137/090771806>`
    and also
    :doi:`Martinsson, P. G., Rokhlin, V., and Tygert, M. (2011).
```

```
"A randomized algorithm for the decomposition of matrices".
Applied and Computational Harmonic Analysis, 30(1), 47-68.
<10.1016/j.acha.2010.02.003>`

Examples
--------
>>> import numpy as np
>>> from sklearn.decomposition import PCA
>>> X = np.array([[-1, -1], [-2, -1], [-3, -2], [1, 1], [2, 1], [3, 2]])
>>> pca = PCA(n_components=2)
>>> pca.fit(X)
PCA(n_components=2)
>>> print(pca.explained_variance_ratio_)
[0.9924... 0.0075...]
>>> print(pca.singular_values_)
[6.30061... 0.54980...]

>>> pca = PCA(n_components=2, svd_solver='full')
>>> pca.fit(X)
PCA(n_components=2, svd_solver='full')
>>> print(pca.explained_variance_ratio_)
[0.9924... 0.00755...]
>>> print(pca.singular_values_)
[6.30061... 0.54980...]

>>> pca = PCA(n_components=1, svd_solver='arpack')
>>> pca.fit(X)
PCA(n_components=1, svd_solver='arpack')
>>> print(pca.explained_variance_ratio_)
[0.99244...]
>>> print(pca.singular_values_)
[6.30061...]
File:           c:\users\hp\appdata\local\programs\python\python312\lib\site-package
s\sklearn\decomposition\_pca.py
Type:           ABCMeta
Subclasses:
```

In [33]:
```python
pca = PCA(n_components=13)
pca
```

Out[33]:
```
▾ PCA
PCA(n_components=13)
```

In [34]:
```python
pca.fit(X_train)
```

Out[34]:
```
▾ PCA
PCA(n_components=13)
```

In [35]:
```python
pca.explained_variance_ratio_
```

```
Out[35]:  array([0.36191771, 0.19946694, 0.11217017, 0.07067914, 0.05928309,
                 0.05403732, 0.04128999, 0.02830445, 0.02076498, 0.01843724,
                 0.01297146, 0.01226998, 0.00840752])
```

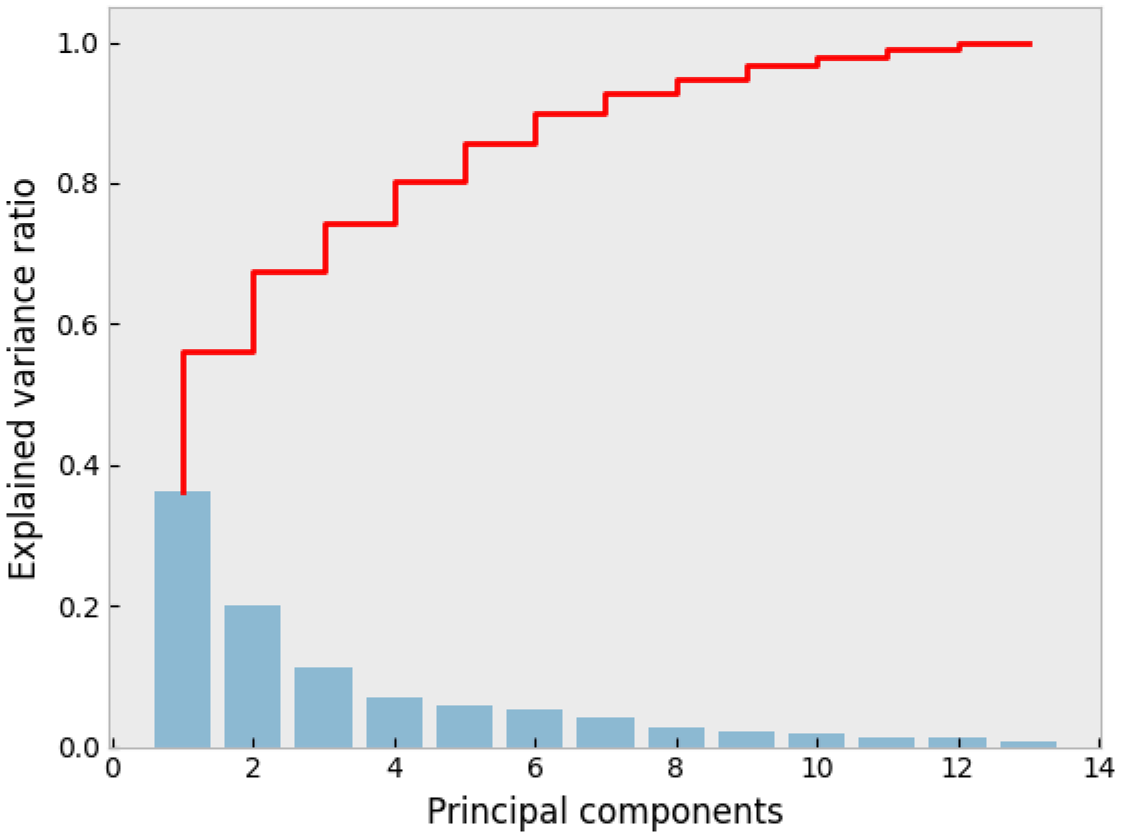
```
In [36]: np.cumsum(pca.explained_variance_ratio_)
```

```
Out[36]:  array([0.36191771, 0.56138466, 0.67355483, 0.74423397, 0.80351705,
                 0.85755438, 0.89884437, 0.92714882, 0.9479138 , 0.96635104,
                 0.9793225 , 0.99159248, 1.        ])
```

```
In [37]: # The matrix A = U.T is
         pca.components_.shape, #MxD
```

```
Out[37]:  ((13, 13),)
```

```
In [38]: plt.step(range(1,14),np.cumsum(pca.explained_variance_ratio_),c='r')
         plt.bar(range(1,14),pca.explained_variance_ratio_, alpha=0.5)
         plt.ylabel('Explained variance ratio')
         plt.xlabel('Principal components');
```



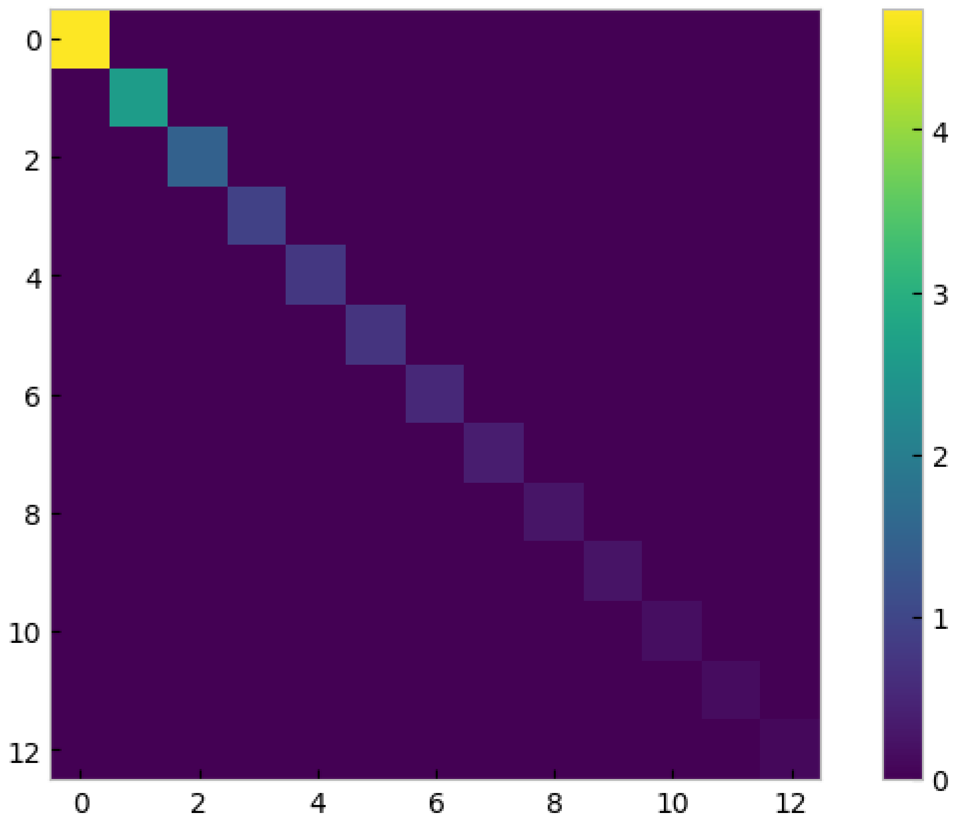
```
In [ ]:
```

```
In [ ]:
```

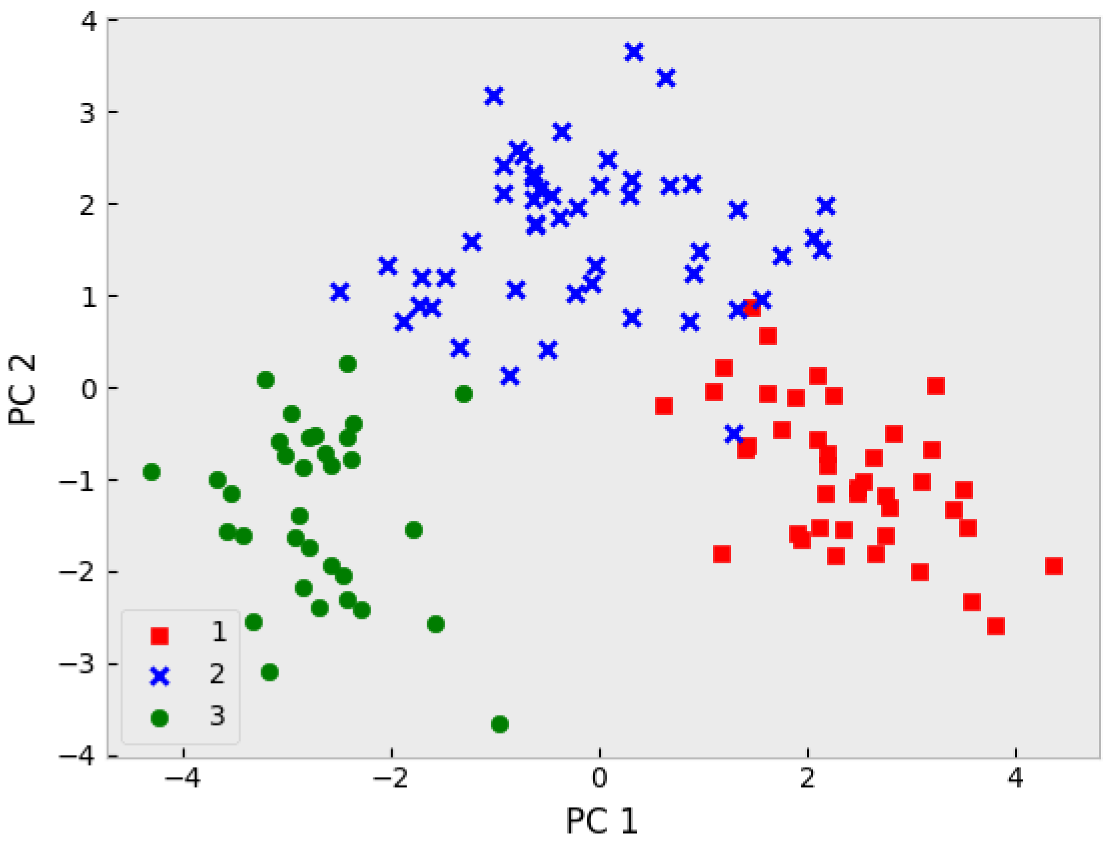
```
In [39]: y_train_pca = pca.transform(X_train)

         y_train_pca.shape
```

```
Out[39]: (124, 13)
```

```
In [40]: cov_mat = np.cov(y_train_pca.T)

         plt.figure(figsize=(8,5))
         plt.imshow(cov_mat)
         plt.colorbar();
```



```
In [41]: colors = ['r', 'b', 'g']
         markers = ['s', 'x', 'o']

         for l, c, m in zip(np.unique(t_train), colors, markers):
             plt.scatter(y_train_pca[t_train==l, 0], y_train_pca[t_train==l, 1],c=c, label=l

         plt.xlabel('PC 1')
         plt.ylabel('PC 2')
         plt.legend(loc='lower left')
         plt.show()
```



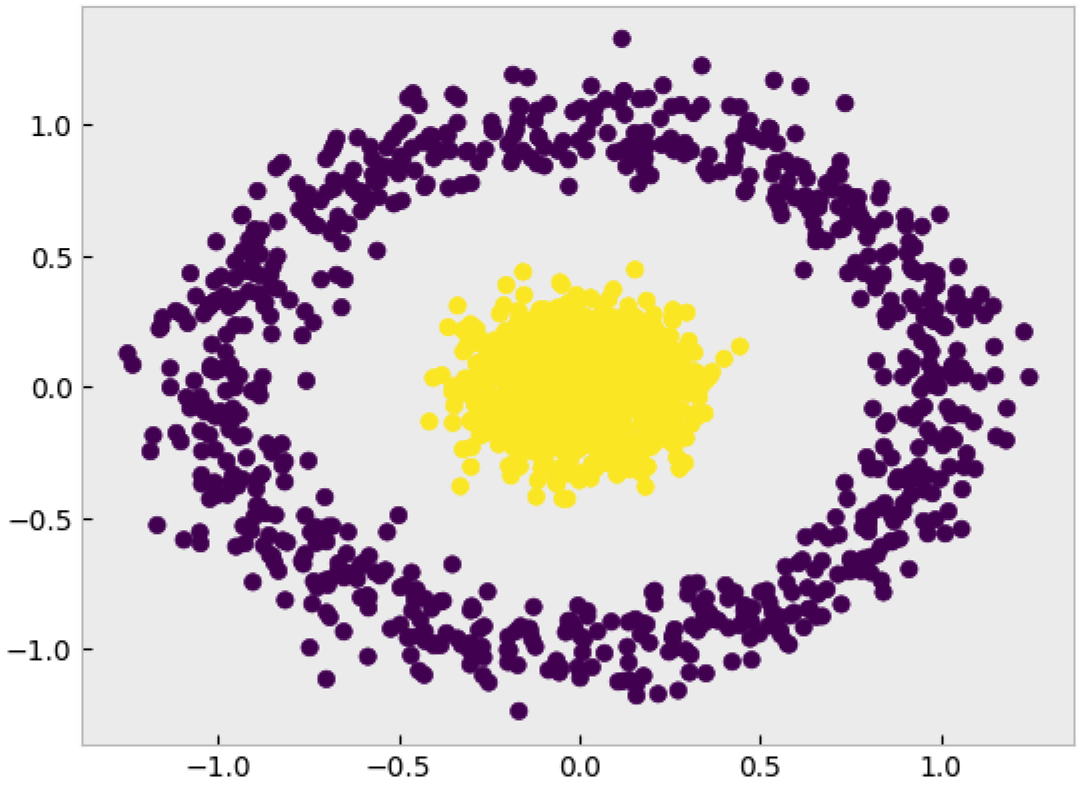
The training data is used to find the new features (eigenvectors). We can then represent the test set in this new feature space:

In [42]:
```
y_test_pca = pca.transform(X_test)

y_test_pca.shape
```

Out[42]:
```
(54, 13)
```

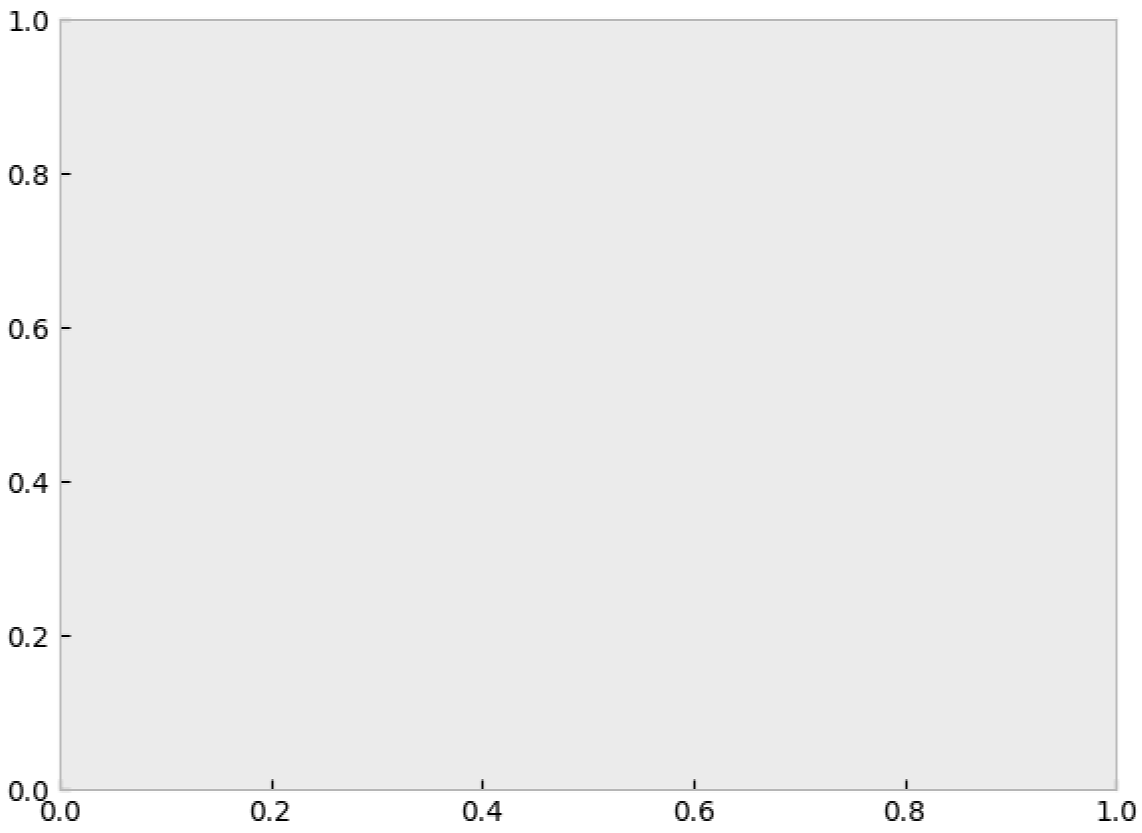
Example: Concentric Circles

In [43]:
```
from sklearn.datasets import make_circles

X, y = make_circles(n_samples=1500, noise=0.1, factor=0.2)

plt.scatter(X[:,0],X[:,1],c=y);
```



In [65]:
```
pca = PCA(n_components = 2)
X_spca = pca.fit_transform(X)

plt.figure(figsize=(15,5))
plt.subplot(1,2,1)
plt.scatter(X_spca[:,0], X_spca[:,1], c=y, alpha=0.5)
plt.subplot(1,2,2)
plt.scatter(X_spca[:,0], np.zeros(len(X_spca[:,0])), c=y, alpha=0.5)
plt.xlabel('PC1');
```

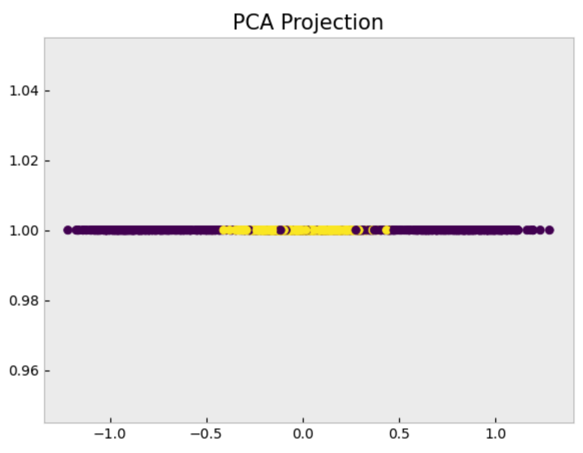
```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\axes\_axes.py:4486, in Axes._parse_scatter_color_args(c, edgecolors, kwargs, xsiz
e, get_next_color_func)
   4485 try:  # Is 'c' acceptable as PathCollection facecolors?
-> 4486     colors = mcolors.to_rgba_array(c)
   4487 except (TypeError, ValueError) as err:

File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\colors.py:505, in to_rgba_array(c, alpha)
    504 else:
--> 505     rgba = np.array([to_rgba(cc) for cc in c])
    507 if alpha is not None:

File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\colors.py:302, in to_rgba(c, alpha)
    301 if rgba is None:  # Suppress exception chaining of cache lookup failure.
--> 302     rgba = _to_rgba_no_colorcycle(c, alpha)
    303     try:

File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\colors.py:391, in _to_rgba_no_colorcycle(c, alpha)
    390 if not np.iterable(c):
--> 391     raise ValueError(f"Invalid RGBA argument: {orig_c!r}")
    392 if len(c) not in [3, 4]:

ValueError: Invalid RGBA argument: 1.0

The above exception was the direct cause of the following exception:

ValueError                                Traceback (most recent call last)
Cell In[65], line 6
      4 plt.figure(figsize=(15,5))
      5 plt.subplot(1,2,1)
----> 6 plt.scatter(X_spca[:,0], X_spca[:,1], c=y, alpha=0.5)
      7 plt.subplot(1,2,2)
      8 plt.scatter(X_spca[:,0], np.zeros(len(X_spca[:,0])), c=y, alpha=0.5)

File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\pyplot.py:3699, in scatter(x, y, s, c, marker, cmap, norm, vmin, vmax, alpha, line
widths, edgecolors, plotnonfinite, data, **kwargs)
   3680 @_copy_docstring_and_deprecators(Axes.scatter)
   3681 def scatter(
   3682     x: float | ArrayLike,
   (...)
   3697     **kwargs,
   3698 ) -> PathCollection:
-> 3699     __ret = gca().scatter(
   3700         x,
   3701         y,
   3702         s=s,
   3703         c=c,
   3704         marker=marker,
   3705         cmap=cmap,
   3706         norm=norm,
   3707             vmin=vmin,
   3708             vmax=vmax,
   3709             alpha=alpha,
   3710             linewidths=linewidths,
   3711             edgecolors=edgecolors,
   3712             plotnonfinite=plotnonfinite,
   3713             **({"data": data} if data is not None else {}),
   3714             **kwargs,
   3715         )
   3716     sci(__ret)
   3717     return __ret

File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\__init__.py:1478, in _preprocess_data.<locals>.inner(ax, data, *args, **kwargs)
   1475 @functools.wraps(func)
   1476 def inner(ax, *args, data=None, **kwargs):
   1477     if data is None:
-> 1478         return func(ax, *map(sanitize_sequence, args), **kwargs)
   1480     bound = new_sig.bind(ax, *args, **kwargs)
   1481     auto_label = (bound.arguments.get(label_namer)
   1482                   or bound.kwargs.get(label_namer))

File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\axes\_axes.py:4673, in Axes.scatter(self, x, y, s, c, marker, cmap, norm, vmin, vm
ax, alpha, linewidths, edgecolors, plotnonfinite, **kwargs)
   4670 if edgecolors is None:
   4671     orig_edgecolor = kwargs.get('edgecolor', None)
   4672 c, colors, edgecolors = \
-> 4673     self._parse_scatter_color_args(
   4674         c, edgecolors, kwargs, x.size,
   4675         get_next_color_func=self._get_patches_for_fill.get_next_color)
   4677 if plotnonfinite and colors is None:
   4678     c = np.ma.masked_invalid(c)

File c:\Users\HP\AppData\Local\Programs\Python\Python312\Lib\site-packages\matplotli
b\axes\_axes.py:4492, in Axes._parse_scatter_color_args(c, edgecolors, kwargs, xsiz
e, get_next_color_func)
   4490 else:
   4491     if not valid_shape:
-> 4492         raise invalid_shape_exception(c.size, xsize) from err
   4493     # Both the mapping *and* the RGBA conversion failed: pretty
   4494     # severe failure => one may appreciate a verbose feedback.
   4495     raise ValueError(
   4496         f"'c' argument must be a color, a sequence of colors, "
   4497         f"or a sequence of numbers, not {c!r}") from err

ValueError: 'c' argument has 1500 elements, which is inconsistent with 'x' and 'y' w
ith size 400.
```

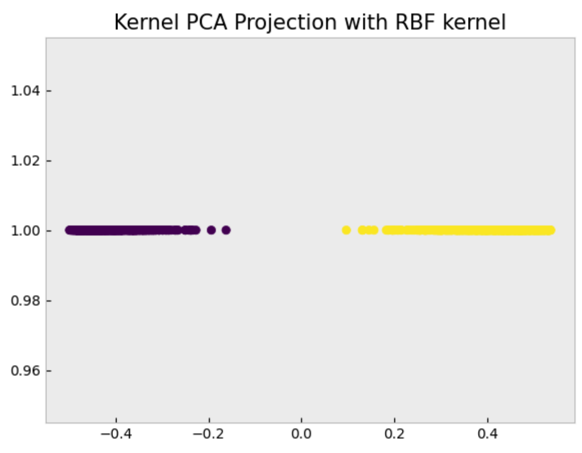


Kernel PCA

There are other variants of PCA such as **Kernel PCA**, where we first project the data to a space where classes are linearly separable (RBF kernel) and then apply PCA:

In [45]:
```
from sklearn.decomposition import KernelPCA

model_pca = PCA(n_components=1)
proj = model_pca.fit_transform(X)

model_kpca = KernelPCA(n_components=1,kernel='rbf',gamma=2)
proj_kpca = model_kpca.fit_transform(X)

plt.figure(figsize=(15,5))
plt.subplot(121); plt.scatter(proj,np.ones(len(proj)),c=y)
plt.title('PCA Projection', size=15)
plt.subplot(122); plt.scatter(proj_kpca,np.ones(len(proj_kpca)),c=y)
plt.title('Kernel PCA Projection with RBF kernel',size=15);
```





Example: Eigenfaces

- Part of this example comes from: http://scikit-learn.org/stable/auto_examples/decomposition/plot_faces_decomposition.html

In [46]:
```
from sklearn.datasets import fetch_olivetti_faces

faces = fetch_olivetti_faces(return_X_y=False)

# print(faces.DESCR)
```

```
downloading Olivetti faces from https://ndownloader.figshare.com/files/5976027 to
C:\Users\HP\scikit_learn_data
```

In [47]:
```
X = faces.data # data matrix

t = faces.target # target label

X.shape, t.shape # 400 images, each of size 64x64=4096 pixels
```

Out[47]:
```
((400, 4096), (400,))
```

In [48]:
```
fig = plt.figure(figsize=(10,10))
for i in range(40):
    fig.add_subplot(7,6,i+1)
    idx = np.random.choice(np.where(t==i)[0])
    plt.imshow(X[idx,:].reshape(64,64), cmap='gray')
    plt.axis('off')
```

```
In [49]: np.unique(t, return_counts=True)
```

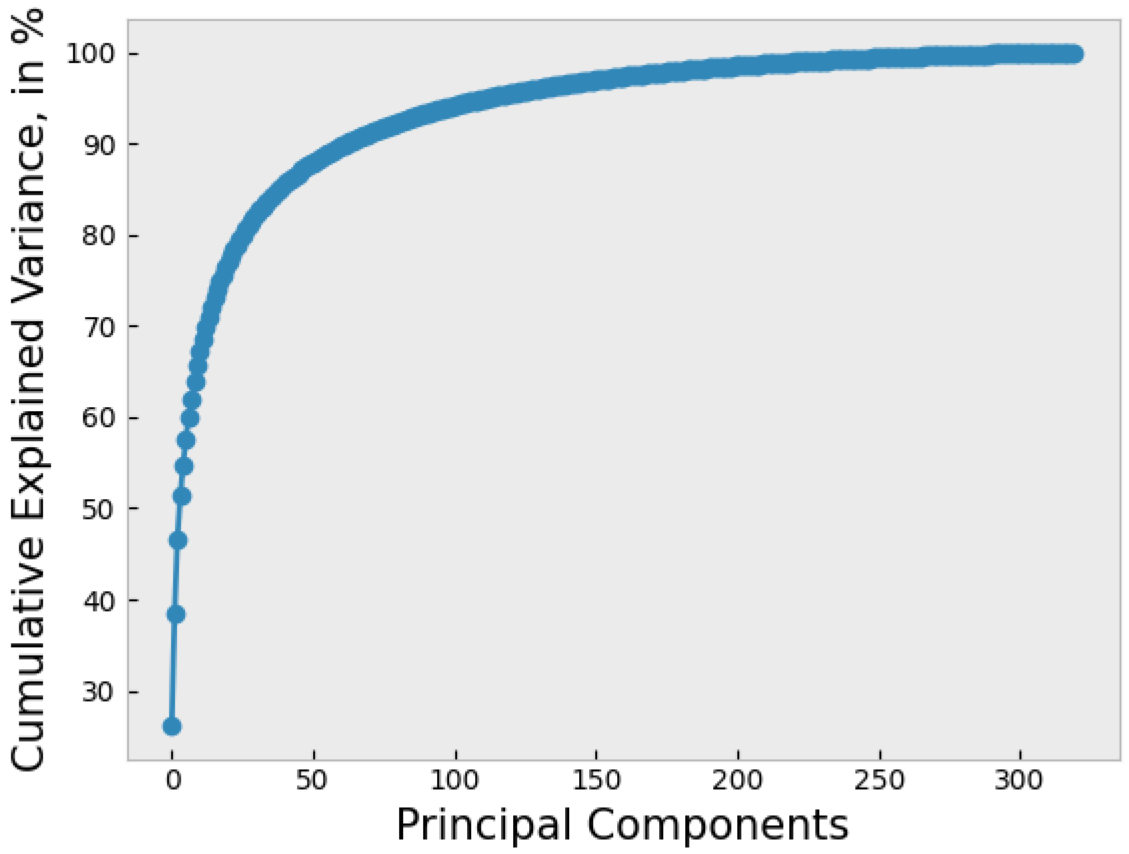
```
Out[49]: (array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16,
                 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33,
                 34, 35, 36, 37, 38, 39]),
          array([10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10,
                 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10,
                 10, 10, 10, 10, 10, 10], dtype=int64))
```

```
In [50]: from sklearn.model_selection import train_test_split

         X_train, X_test, t_train, t_test = train_test_split(X, t,
                                                             test_size=0.2,
                                                             random_state=42)

         X_train.shape, t_train.shape, X_test.shape, t_test.shape
```

```
Out[50]: ((320, 4096), (320,), (80, 4096), (80,))
```

```
In [51]: scaler = StandardScaler()
         X_train_scaled = scaler.fit_transform(X_train)
         X_test_scaled = scaler.transform(X_test)
```

```
In [52]: pca = PCA(n_components=320)
         pca.fit_transform(X_train_scaled);

         plt.plot(100*np.cumsum(pca.explained_variance_ratio_), '-o')
         plt.xlabel('Principal Components',size=15)
         plt.ylabel('Cumulative Explained Variance, in %', size=15);
```



```
In [53]: np.where(np.cumsum(pca.explained_variance_ratio_)>=0.9)
```

```
Out[53]: (array([ 62,  63,  64,  65,  66,  67,  68,  69,  70,  71,  72,  73,  74,
                  75,  76,  77,  78,  79,  80,  81,  82,  83,  84,  85,  86,  87,
                  88,  89,  90,  91,  92,  93,  94,  95,  96,  97,  98,  99, 100,
                 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113,
                 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126,
                 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139,
                 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152,
                 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165,
                 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178,
                 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191,
                 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204,
                 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217,
                 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230,
                 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243,
                 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256,
                 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269,
                 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282,
                 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295,
                 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308,
                 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319], dtype=int64),)
```

```
In [ ]:
```

```
In [ ]:
```

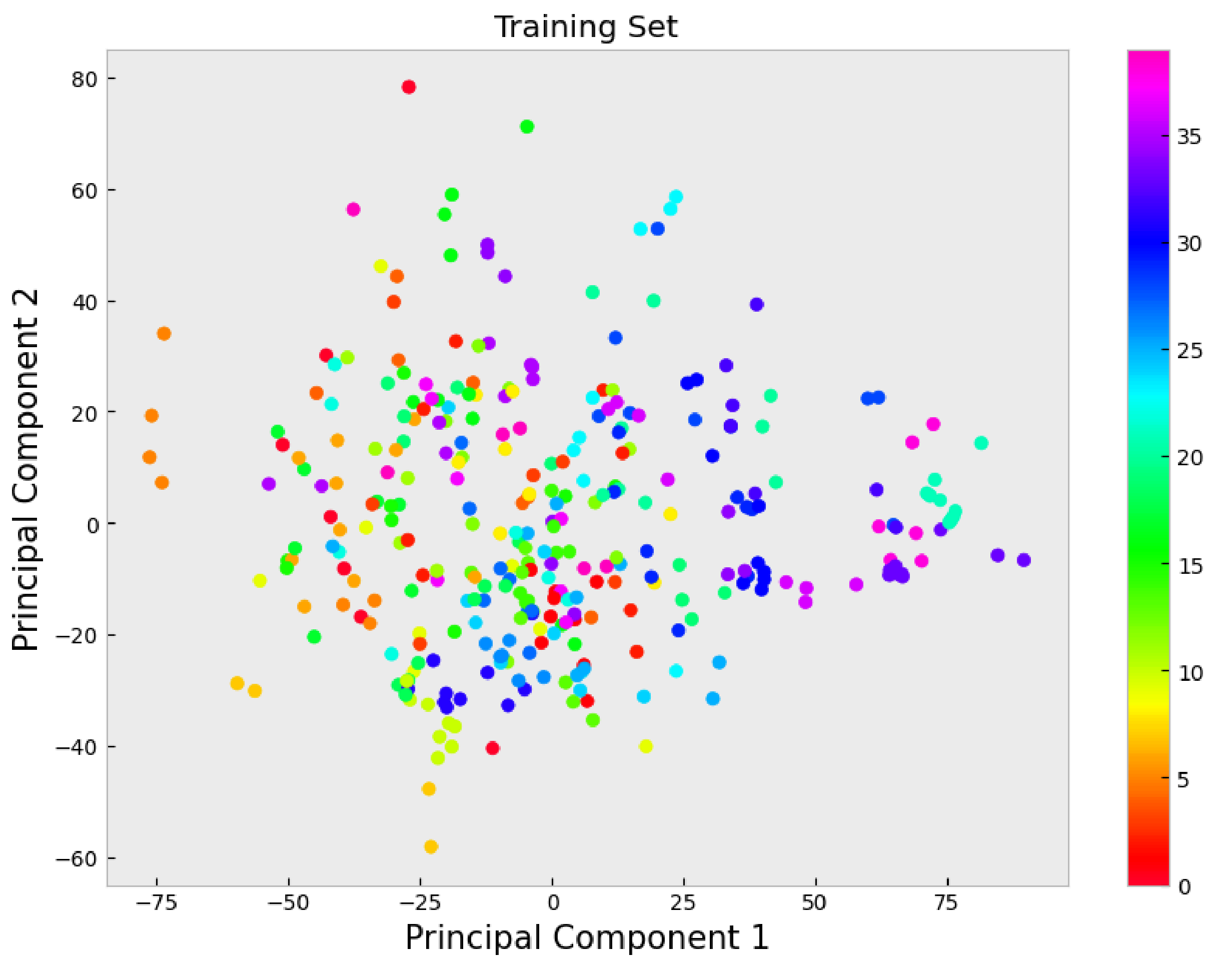
In order to explain 90% of the variance in the data, we need to preserve 63 principal components.

Let's project to 2-D so we can plot it:

```
In [54]: pca = PCA(n_components=2)
         ypca = pca.fit_transform(X_train_scaled)

         ypca.shape
```

```
Out[54]: (320, 2)
```

```
In [55]: plt.figure(figsize=(10,7))
         plt.scatter(ypca[:,0], ypca[:,1], c=t_train, cmap=plt.cm.gist_rainbow)
         plt.xlabel('Principal Component 1', size=15)
         plt.ylabel('Principal Component 2', size=15)
         plt.title('Training Set')
         plt.colorbar();
```



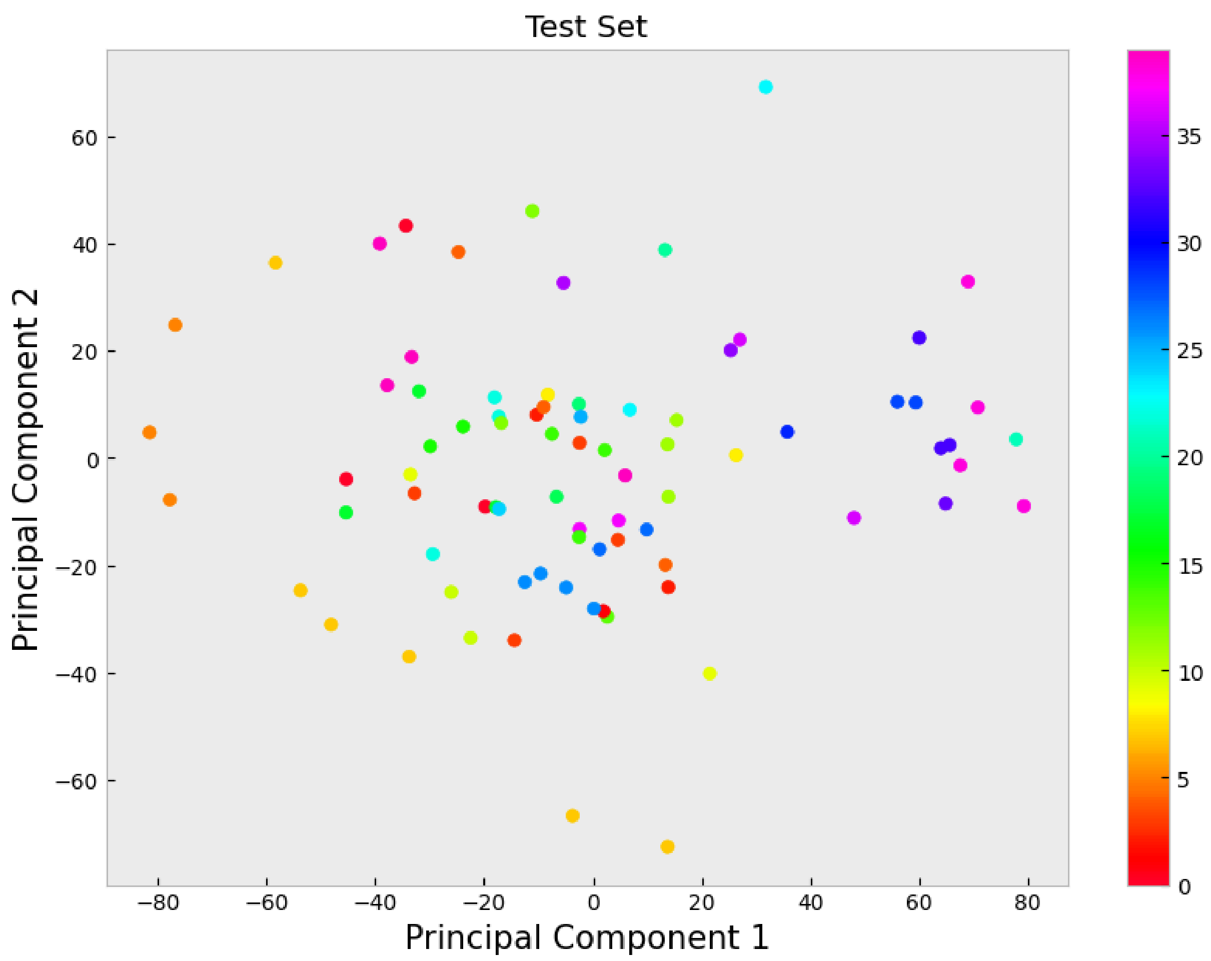
Not that the 40 classes are overlapping in the linear projection space. This is because PCA is **unsupervised**, it does use the class labels *anywhere* in finding the matrix for linear projection.

To apply this transformation in the test set, simply multiply the resultant modal matrix with the scaled test set:

In [56]:
```
# Transform the test set using the linear transformation found with the training da
ypca_test = pca.transform(X_test_scaled)

ypca_test.shape
```

Out[56]:
```
(80, 2)
```

In [57]:
```
plt.figure(figsize=(10,7))
plt.scatter(ypca_test[:,0], ypca_test[:,1], c=t_test, cmap=plt.cm.gist_rainbow)
plt.xlabel('Principal Component 1', size=15)
plt.ylabel('Principal Component 2', size=15)
plt.title('Test Set')
plt.colorbar();
```



You can access the linear transformation $\mathbf{A} = \mathbf{U}^T$ using the method `components_`:

```
In [58]: A = pca.components_

         A.shape
```

```
Out[58]: (2, 4096)
```

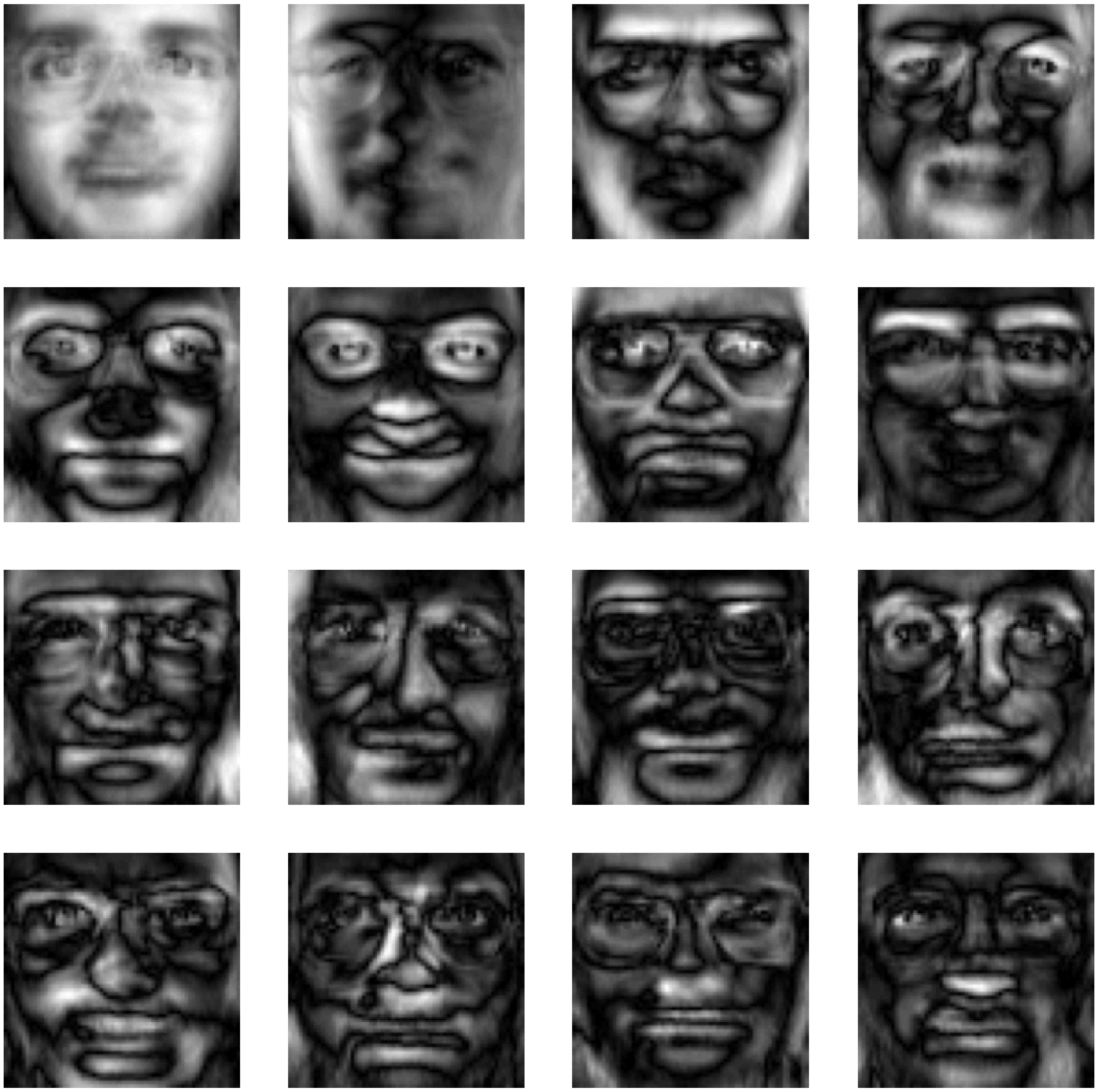
Note that the eigenvectors are described in the original space, that is, they are 4096-dimensional!

Since we are working with images, we can reshape them back to a 64×64 image and see what are the regions in the image with maximum explained variance! This is called the **eigenfaces**.

Let's now recover 16 eigenvectors and plot them as images:

```
In [66]: n_components = 16

         pca = PCA(n_components=n_components)
         ypca = pca.fit_transform(X_train_scaled)

         fig=plt.figure(figsize=(10,10))
         for i in range(n_components):
```

```
    fig.add_subplot(4,4,i+1)
    plt.imshow(abs(pca.components_[i,:].reshape(64,64)),cmap='gray')
    plt.axis('off')
```



The eigenvectors are describing the regions in the 64x64 image that explain the most variance. the more eigenvectors are kept, the better a reconstruction image will be produced.

Since the projection is given by:

$$\mathbf{Y} = \mathbf{A}\mathbf{X}$$

In order to recover $\mathbf{X}$, we need to left-multiply by the pseudo-inverse of $\mathbf{A}$:

$$\hat{\mathbf{X}} = \mathbf{A}^{\dagger}\mathbf{Y}$$

We'll code this up next class.