04_dimensionality_reduction

April 7, 2022

1 Unsupervised Learning: dimensionality reduction

2 Outline

1. Section **??**
2. Section **??**
3. Section **??**
4. Section **??**
5. Section **??**
6. Section **??**

[1]:
```
from IPython.display import Image
import matplotlib.pyplot as plt
import numpy as np
import random
import scipy as sp
import sklearn.metrics as skmetrics

import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib.ticker import NullFormatter
```

2.1 Recap: what is Unsupervised Learning

Supervised learning: discover patterns relating data attributes (descriptors, features) with a target (class) attribute → create a model. The model is used to predict the values of the target attribute in future data instances.

Unsupervised learning: The data have no target attribute → we want to explore the data to find some intrinsic structures in them: - Learn new features - Learn groupings

Many example data sets and techniques provided by SciKit-Learn

2.2 Measuring features

We use the terms *features*, *coordinates*, *attributes* as synonims

We use the terms *distance* or *dissimilarity* as synonims and as the opposite of *similarity*

There are numerous distance functions for - Different types of data - Numeric data - Nominal data - Different specific applications

2.2.1 Numeric attributes

The most commonly used distances are the: - L_2 norm, i. e. the Euclidean distance - L_1 norm called also *cityblock* or *Manhattan* distance

L_1 and L_2 are a special case of *Minkowski* distance where h is positive integer:

$$d(x_i, x_j) = \left(\sum_1^f (x_{if} - x_{jf}) \right)^{\frac{1}{h}}$$

L_∞ norm called also *Chebyshev distance* or *supremum distance* and defined as

$$d(x_i, x_j) = max_{i,j}|x_i - x_j|$$

it is the limit of the above definition for $h \to \infty$; one wants to define two data points as "different" if they are different on any one of the attributes

Any definition of distance can be weighted:

$$d(x_i, x_j) = \left(\sum_1^f w_f(x_{if} - x_{jf}) \right)^{\frac{1}{h}}$$

2.2.2 Binary or nominal features

A binary attribute is *symmetric* if both of its states (0 and 1) have equal importance, and carry the same weights, e.g., even or odd.
Simple matching function proportion of mismatches of their values

$$dist(x_i, x_j) = \frac{b + c}{a + b + c + d}$$

Example:

$$x_1 = (1, 1, 1, 0, 1, 0, 0)$$
$$x_2 = (0, 1, 1, 0, 0, 1, 0)$$
$$d_{x_1,x_2} = \frac{2 + 1}{2 + 2 + 1 + 2} = \frac{3}{7}$$

2.2.3 Jaccard coefficent

Asymmetric attribute: if one of the states is more important or more valuable than the other. State 1 *usually* represents the more important state, which is typically the rare or infrequent state. Jaccard coefficient:

$$dist(x_i, x_j) = \frac{b + c}{a + b + c}$$

2.2.4 Hamming distance

for two strings of equal length is the number mismatches in the same position:

$$x_1 = (1, 1, 1, 0, 1, 0, 0)$$
$$x_2 = (0, 1, 1, 0, 0, 1, 0)$$
$$d_{x_1,x_2} = 3$$

2.2.5 Mixed features

how can we compute the dissimilarity between objects of mixed attribute types?

simple approach: group each type of attribute together, performing separate data analysis for each type; unfeasible if the features are not distributed in a similar way

Unified distance:

$$dist(x_i, x_j) = \frac{\sum_{f=1}^{h} \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^{h} \delta_{ij}^{(f)}}$$

where: - δ_{ij} is 1 if x_{if} or x_{jf} are missing or are 0 for a *binary symmetric* feature - 1 otherwise
in addition d_{ij} is: - numeric: $d_{ij}^{(f)} = \frac{|x_{if} - x_{jf}}{max x_f - min x_f}$ - nominal or binary: $d_{ij}^{(f)}$ if $x_{if} = x_{jf}$ otherwise 0

2.2.6 Exercise

Write a function to calculate the Hamming distance

2.2.7 Solution

[2]:
```
def hamming(it1, it2):
    """Return the Hamming distance between equal-length iterables."""
    if len(it1) != len(it2):
        raise ValueError("Lengths must be equal!")
    ham = np.sum([item1 !=item2 for item1,item2 in zip(it1,it2)])
    return ham
```

[3]:
```
x_1 = (1,1,1,0,1,0,0)
x_2 = (0,1,1,0,0,1,0)
hamming(x_1,x_2)
```

[3]: 3

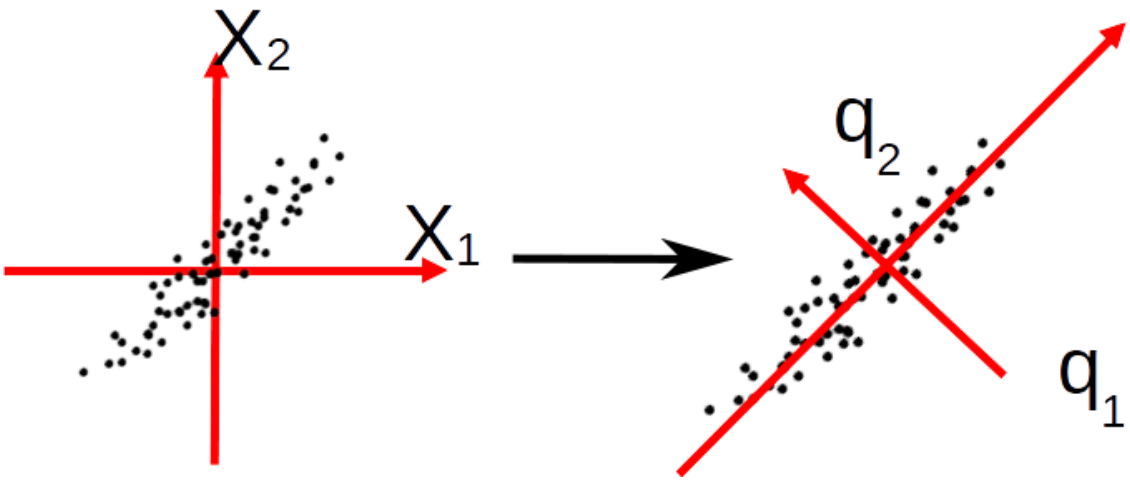
2.3 Dimensionality reduction: motivation

Data compression:

Suppose we have a two variable data set like the one on the left:

[4]:
```
Image(filename="ellipsoid.svg.png")
```

[4]:

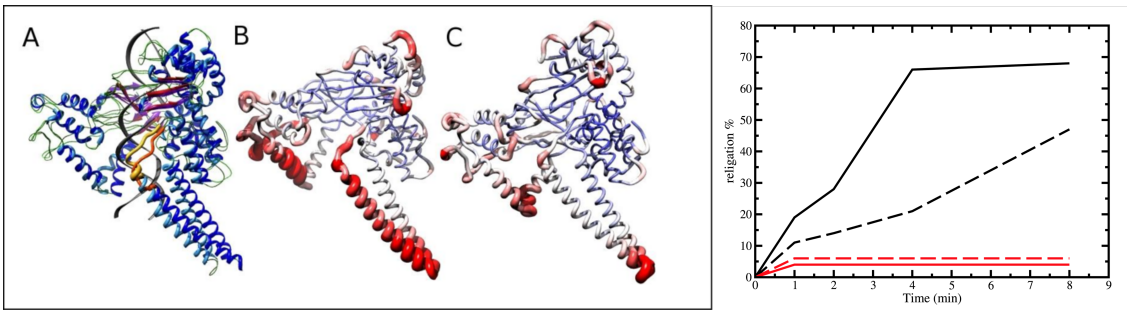


We may want to rotate the laboratory axes to a new set $q1, q2$. Why?

Using x_1, x_2 we see that both independent variables are important to locate a data point in space within an acceptable error. However, in the q_1, q_2 system q_1 would suffice.
We have *reduced the dimensionality* of the system. Remember the *curse of dimensionality*

Data visualization:

[5]:
```
Image(filename="topo.png")
```

[5]:


2.4 Principal component analysis

How can we measure the ``amount of information'' carried by x_1 or x_2 and decide how much to rotate the reference system? We can use their variance:

$$var(x) = \frac{1}{N}\sum_{i=1}^{N}(x - \bar{x})^2$$

A ``useful rotation'' would move part of the variance of $x2$ to $x1$. In doing this we also reduce the covariance between $x1$ and $x2$:

$$cov(x1, x2) = (x1 - \bar{x1})(x2 - \bar{x2})$$

For n independent variables we can calculate the (symmetric) covariance matrix with elements $\Sigma_{ij} = cov(x_i, x_j)$. A good strategy would be then to have *uncorrelated* variables, e.g. by diagonalizing Σ:

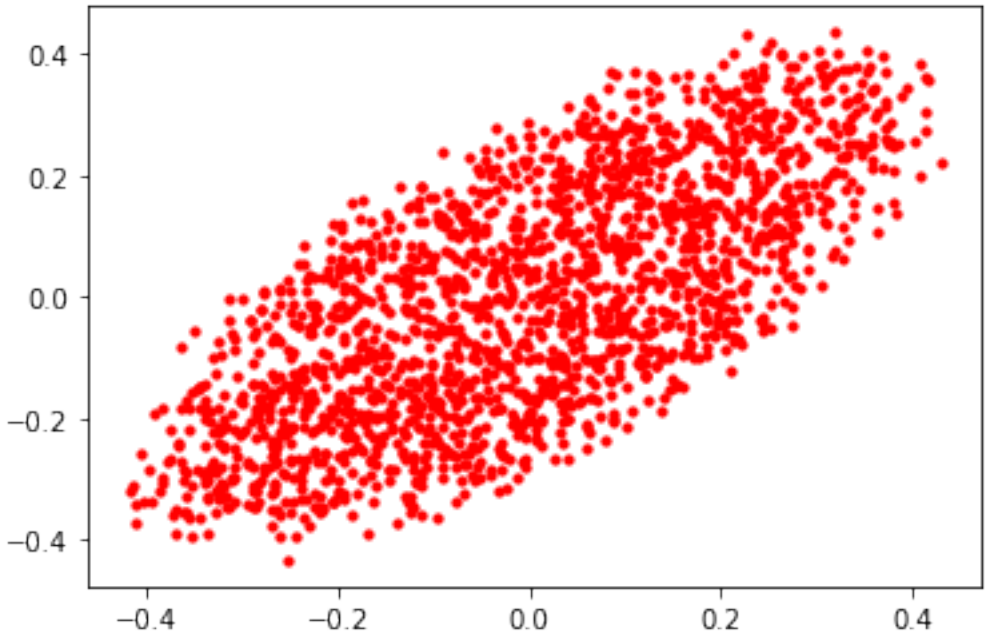
$$U^{-1}\Sigma U = (\lambda_1, \lambda_2, \ldots, \lambda_n)$$

The eigenvalues λ_i will the include the *amount of variance explained* by each eigenvector U_i.

[6]:
```
npoints = int(1e5)
a = 0.8
b = 0.1
#ellipse centered in .0, .0
x = 4*np.random.rand(npoints)-2.
y = 4*np.random.rand(npoints)-2.
r = (7*x)**2+(3*y)**2
sample = r <= 1. + 2*np.random.rand(npoints)
#rotation of the axes
alpha = 45.*(np.pi/180.)
xprime = x[sample]*np.cos(alpha) + y[sample]*np.sin(alpha)
yprime = -x[sample]*np.sin(alpha) + y[sample]*np.cos(alpha)
```

[7]:
```
plt.scatter(xprime,yprime,marker='o',s=10,color='r')
```

[7]:
```
<matplotlib.collections.PathCollection at 0x7f149af95bb0>
```



Ordinating the eigenvalues and choosing a number of them equals to project the data set on a subspace whose vectors are those correspoding to the highest explained variance. This is what **Principal Component Analysis** (Pearson 1901, Hotelling 1933) does.

[8]:
```
from sklearn.decomposition import PCA
data = np.vstack((xprime,yprime)).T
estimator = PCA(n_components=2)
estimator.fit(data)
print(estimator.explained_variance_ratio_,np.sum(estimator.
 ↪explained_variance_ratio_))
print(estimator.components_)
```

```
[0.8562642 0.1437358] 1.0
[[ 0.70175232  0.712421  ]
 [-0.712421    0.70175232]]
```

Thus the $q1$ variable explains approximately 85% of the total variance.

PCA is useful if data is contained in an ellipsoid; however if I have a 4D hypersphere:

[9]:
```
npoints = int(1e5)
w = 2*np.random.rand(npoints)-1.
x = 2*np.random.rand(npoints)-1.
y = 2*np.random.rand(npoints)-1.
z = 2*np.random.rand(npoints)-1.
r = w**2 + x**2 + y**2 + z**2
inside = r<1.
data = np.vstack((w[inside],x[inside],y[inside],z[inside])).T
mypca = PCA(n_components=4)
mypca.fit(data)
print(mypca.explained_variance_ratio_,np.sum(mypca.explained_variance_ratio_))
```

```
[0.25288052 0.25200899 0.24877119 0.2463393 ] 1.0
```

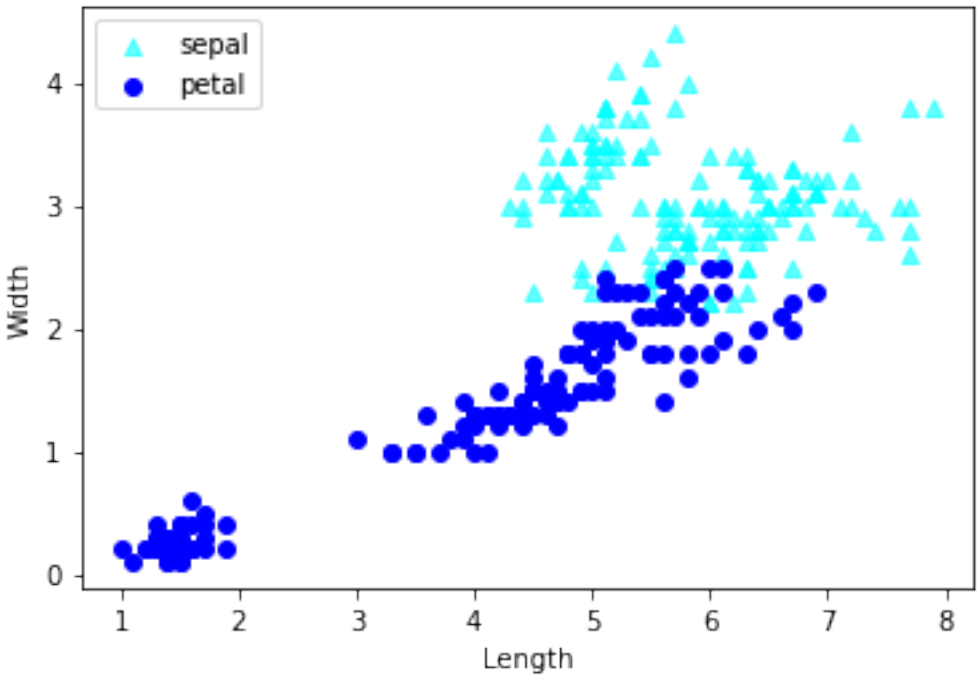
2.4.1 Example: Iris data set

[10]:
```
from sklearn import datasets

iris = datasets.load_iris()
X = iris.data
Y = iris.target
```

Plot sepals vs petals:

[11]:
```
plt.scatter(X[:, 0], X[:, 1], c='cyan', marker='^',label="sepal",alpha=0.
↪6,edgecolor=None)
plt.scatter(X[:, 2], X[:, 3], c='blue', marker='o',label="petal",edgecolor=None)
plt.xlabel('Length')
plt.ylabel('Width')
plt.legend()
```

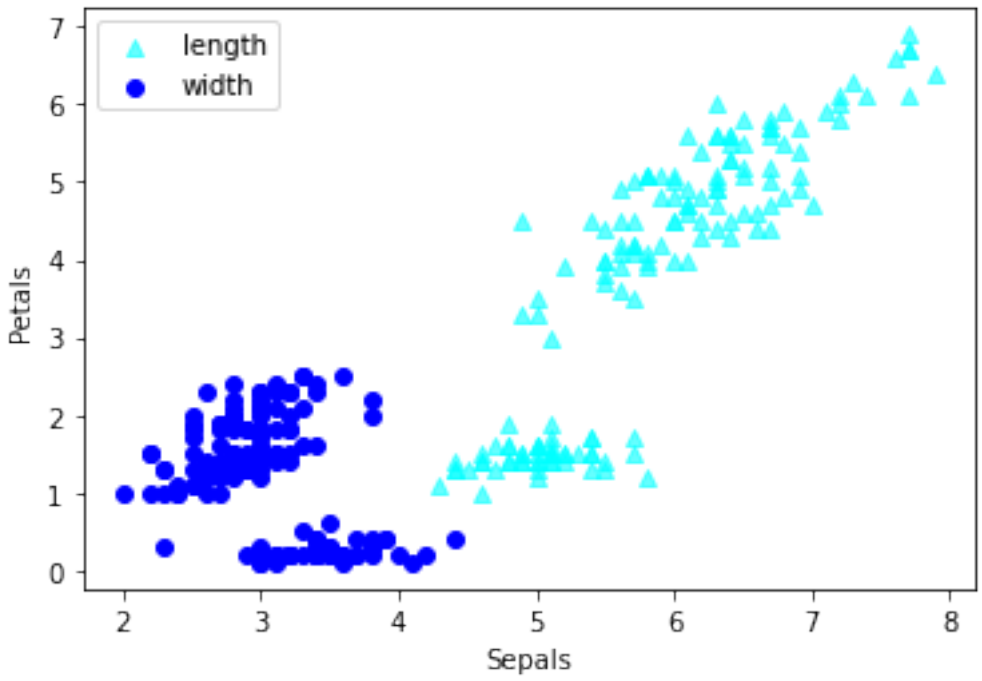
[11]: <matplotlib.legend.Legend at 0x7f1498032ca0>



Compare lenght and width

[12]:
```
plt.scatter(X[:, 0], X[:, 2], c='cyan', marker='^',label="length",alpha=0.6)
plt.scatter(X[:, 1], X[:, 3], c='blue', marker='o',label="width")
plt.xlabel('Sepals')
plt.ylabel('Petals')
plt.legend()
```

[12]: <matplotlib.legend.Legend at 0x7f1498057610>



Before trying PCA, apply *feature scaling*

[13]:
```
import sklearn.preprocessing
from sklearn.decomposition import PCA
Xscaled = sklearn.preprocessing.scale(X)
np.mean(Xscaled),np.var(Xscaled),Xscaled.shape,X.shape
```

[13]:
```
(-1.4684549872375404e-15, 1.0, (150, 4), (150, 4))
```

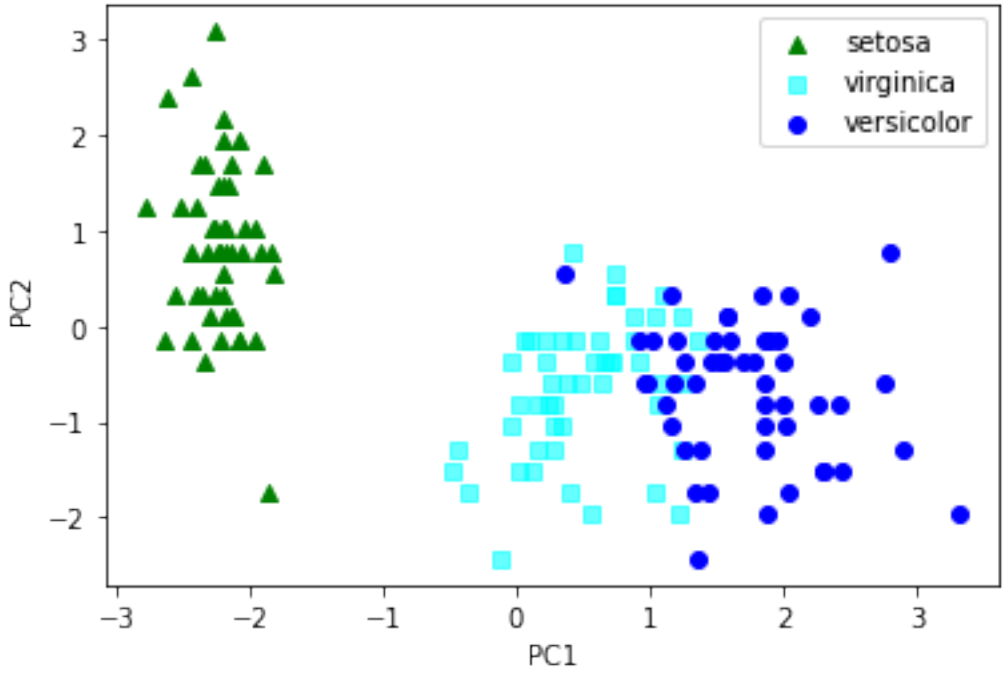
[14]:
```
#create a pca instance
estimator = PCA(n_components=2)
estimator.fit(Xscaled)
X_2d = estimator.fit_transform(Xscaled)
print("Eigenvalues ",estimator.explained_variance_ratio_)
print("Eigenvectors ",estimator.components_)
print("Explained variance ",np.sum(estimator.explained_variance_ratio_))
print("New features",X_2d.shape)
```

```
Eigenvalues  [0.72962445 0.22850762]
Eigenvectors  [[ 0.52106591 -0.26934744  0.5804131   0.56485654]
 [ 0.37741762  0.92329566  0.02449161  0.06694199]]
Explained variance  0.9581320720000165
New features (150, 2)
```

the decomposition seems to be working; let's see how the flowers distribute along the PCs:

[15]:
```
plt.scatter(X_2d[Y==0][:, 0], Xscaled[Y==0][:, 1], c='green',␣
 ↪marker='^',label="setosa")
plt.scatter(X_2d[Y==1][:, 0], Xscaled[Y==1][:, 1], c='cyan',␣
 ↪marker='s',label="virginica",alpha=0.6)
plt.scatter(X_2d[Y==2][:, 0], Xscaled[Y==1][:, 1], c='blue',␣
 ↪marker='o',label="versicolor")
plt.xlabel('PC1')
plt.ylabel('PC2')
plt.legend()
```

[15]:
```
<matplotlib.legend.Legend at 0x7f148e7af3a0>
```



2.4.2 Exercise

Implement a numpy version of PCA and reconstruct an approximation of the original data iris data set from the PC

2.4.3 Solution

[16]:
```
from scipy.linalg import eigh
help(eigh)
```

```
Help on function eigh in module scipy.linalg.decomp:

eigh(a, b=None, lower=True, eigvals_only=False, overwrite_a=False,
```

```
overwrite_b=False, turbo=True, eigvals=None, type=1, check_finite=True,
subset_by_index=None, subset_by_value=None, driver=None)
    Solve a standard or generalized eigenvalue problem for a complex
    Hermitian or real symmetric matrix.

    Find eigenvalues array ``w`` and optionally eigenvectors array ``v`` of
    array ``a``, where ``b`` is positive definite such that for every
    eigenvalue  (i-th entry of w) and its eigenvector ``vi`` (i-th column of
    ``v``) satisfies::

                        a @ vi =  * b @ vi
        vi.conj().T @ a @ vi =
        vi.conj().T @ b @ vi = 1

    In the standard problem, ``b`` is assumed to be the identity matrix.

    Parameters
    ----------
    a : (M, M) array_like
        A complex Hermitian or real symmetric matrix whose eigenvalues and
        eigenvectors will be computed.
    b : (M, M) array_like, optional
        A complex Hermitian or real symmetric definite positive matrix in.
        If omitted, identity matrix is assumed.
    lower : bool, optional
        Whether the pertinent array data is taken from the lower or upper
        triangle of ``a`` and, if applicable, ``b``. (Default: lower)
    eigvals_only : bool, optional
        Whether to calculate only eigenvalues and no eigenvectors.
        (Default: both are calculated)
    subset_by_index : iterable, optional
        If provided, this two-element iterable defines the start and the end
        indices of the desired eigenvalues (ascending order and 0-indexed).
        To return only the second smallest to fifth smallest eigenvalues,
        ``[1, 4]`` is used. ``[n-3, n-1]`` returns the largest three. Only
        available with "evr", "evx", and "gvx" drivers. The entries are
        directly converted to integers via ``int()``.
    subset_by_value : iterable, optional
        If provided, this two-element iterable defines the half-open interval
        ``(a, b]`` that, if any, only the eigenvalues between these values
        are returned. Only available with "evr", "evx", and "gvx" drivers. Use
        ``np.inf`` for the unconstrained ends.
    driver: str, optional
        Defines which LAPACK driver should be used. Valid options are "ev",
        "evd", "evr", "evx" for standard problems and "gv", "gvd", "gvx" for
        generalized (where b is not None) problems. See the Notes section.
    type : int, optional
        For the generalized problems, this keyword specifies the problem type
```

```
    to be solved for ``w`` and ``v`` (only takes 1, 2, 3 as possible
    inputs)::

        1 =>     a @ v = w @ b @ v
        2 => a @ b @ v = w @ v
        3 => b @ a @ v = w @ v

    This keyword is ignored for standard problems.
overwrite_a : bool, optional
    Whether to overwrite data in ``a`` (may improve performance). Default
    is False.
overwrite_b : bool, optional
    Whether to overwrite data in ``b`` (may improve performance). Default
    is False.
check_finite : bool, optional
    Whether to check that the input matrices contain only finite numbers.
    Disabling may give a performance gain, but may result in problems
    (crashes, non-termination) if the inputs do contain infinities or NaNs.
turbo : bool, optional
    *Deprecated since v1.5.0, use ``driver=gvd`` keyword instead*.
    Use divide and conquer algorithm (faster but expensive in memory, only
    for generalized eigenvalue problem and if full set of eigenvalues are
    requested.). Has no significant effect if eigenvectors are not
    requested.
eigvals : tuple (lo, hi), optional
    *Deprecated since v1.5.0, use ``subset_by_index`` keyword instead*.
    Indexes of the smallest and largest (in ascending order) eigenvalues
    and corresponding eigenvectors to be returned: 0 <= lo <= hi <= M-1.
    If omitted, all eigenvalues and eigenvectors are returned.

Returns
-------
w : (N,) ndarray
    The N (1<=N<=M) selected eigenvalues, in ascending order, each
    repeated according to its multiplicity.
v : (M, N) ndarray
    (if ``eigvals_only == False``)

Raises
------
LinAlgError
    If eigenvalue computation does not converge, an error occurred, or
    b matrix is not definite positive. Note that if input matrices are
    not symmetric or Hermitian, no error will be reported but results will
    be wrong.

See Also
--------
```

```
eigvalsh : eigenvalues of symmetric or Hermitian arrays
eig : eigenvalues and right eigenvectors for non-symmetric arrays
eigh_tridiagonal : eigenvalues and right eiegenvectors for
    symmetric/Hermitian tridiagonal matrices

Notes
-----
This function does not check the input array for being hermitian/symmetric
in order to allow for representing arrays with only their upper/lower
triangular parts. Also, note that even though not taken into account,
finiteness check applies to the whole array and unaffected by "lower"
keyword.

This function uses LAPACK drivers for computations in all possible keyword
combinations, prefixed with ``sy`` if arrays are real and ``he`` if
complex, e.g., a float array with "evr" driver is solved via
"syevr", complex arrays with "gvx" driver problem is solved via "hegvx"
etc.

As a brief summary, the slowest and the most robust driver is the
classical ``<sy/he>ev`` which uses symmetric QR. ``<sy/he>evr`` is seen as
the optimal choice for the most general cases. However, there are certain
occassions that ``<sy/he>evd`` computes faster at the expense of more
memory usage. ``<sy/he>evx``, while still being faster than ``<sy/he>ev``,
often performs worse than the rest except when very few eigenvalues are
requested for large arrays though there is still no performance guarantee.


For the generalized problem, normalization with respoect to the given
type argument::

        type 1 and 3 :      v.conj().T @ a @ v = w
        type 2       : inv(v).conj().T @ a @ inv(v) = w

        type 1 or 2  :      v.conj().T @ b @ v  = I
        type 3       : v.conj().T @ inv(b) @ v  = I


Examples
--------
>>> from scipy.linalg import eigh
>>> A = np.array([[6, 3, 1, 5], [3, 0, 5, 1], [1, 5, 6, 2], [5, 1, 2, 2]])
>>> w, v = eigh(A)
>>> np.allclose(A @ v - v @ np.diag(w), np.zeros((4, 4)))
True

Request only the eigenvalues
```

```
    >>> w = eigh(A, eigvals_only=True)

    Request eigenvalues that are less than 10.

    >>> A = np.array([[34, -4, -10, -7, 2],
    …               [-4, 7, 2, 12, 0],
    …               [-10, 2, 44, 2, -19],
    …               [-7, 12, 2, 79, -34],
    …               [2, 0, -19, -34, 29]])
    >>> eigh(A, eigvals_only=True, subset_by_value=[-np.inf, 10])
    array([6.69199443e-07, 9.11938152e+00])

    Request the largest second eigenvalue and its eigenvector

    >>> w, v = eigh(A, subset_by_index=[1, 1])
    >>> w
    array([9.11938152])
    >>> v.shape  # only a single column is returned
    (5, 1)
```

[17]:
```
cov = np.cov(Xscaled.T)/Xscaled.shape[1]
print("cov shape", cov.shape)
myvals, myvecs = eigh(cov)
print(np.sum(myvals))
myvals = myvals[::-1][:2]
myvecs = myvecs.T[::-1][:2]
print(myvals.shape, myvecs.shape)
print(myvals)
print(myvecs)
```

```
cov shape (4, 4)
1.006711409395972
(2,) (2, 4)
[0.73452126 0.23004123]
[[ 0.52106591 -0.26934744  0.5804131   0.56485654]
 [-0.37741762 -0.92329566 -0.02449161 -0.06694199]]
```

[18]:
```
print(X_2d.shape, (myvecs).shape, Xscaled.shape)
Xrec = np.dot(X_2d, myvecs)
print(np.var(Xrec)-np.sum(estimator.explained_variance_ratio_))
```

```
(150, 2) (2, 4) (150, 4)
1.7763568394002505e-15
```

2.4.4 PCA vs Linear Regression

not the same projections

2.4.5 Example: dihedral PCA

Problem: MD simulations of a flexible chromophore, tyrosine. Six torsional degrees of freedom:

Cartesian coordinates do not convey much information on the topology of a flexible molecule. What about using a *dihedral angles*?
Angles are a periodic quantity with circular mean and variance. To deal with it transform from the space of dihedral angles ϕ_n to the coordinate space $x_n = cos\phi_n, y_n = sin\phi_n$ (see Section ??.)

[19]:
```
dih_traj = np.loadtxt("dihedrals.dat")
dih_traj[:10]
```

[19]:
```
array([[-107.475,  -66.147,    3.935,   66.31 ,  -54.5  ,   18.624],
       [-114.625,  -61.6  ,   -5.802,   75.414,  -70.24 ,   -1.611],
       [ -98.298,  -55.725,   17.769,   64.068,  -65.778,    6.477],
       [-142.168,  -74.425,    4.04 ,   54.909,  -67.441,    1.417],
       [-124.6  ,  -72.523,  -17.768,   50.227,  -57.1  ,  -11.357],
       [-155.604,  -64.068,  -17.56 ,   55.1  ,  -58.364,  -20.701],
       [-140.617,  -61.435,    3.72 ,   49.005,  -82.538,    4.522],
       [-171.321,  -74.027,   -1.862,   51.268,  -77.627,  -14.77 ],
       [-159.473,  -58.516,   -7.833,   51.632,  -70.928,    6.393],
       [ 178.378,  -37.398,   18.537,   39.383,  -60.463,   -6.354]])
```

[20]:
```
n_frames=dih_traj.shape[0]
dih_tot=len(dih_traj[0,:])
print("number of frames ",n_frames)
print("number of dihedrals ", dih_tot)
```

```
number of frames  5847
number of dihedrals  6
```

[21]:
```
sinv = np.sin(dih_traj*(np.pi/180.0))
cosv = np.cos(dih_traj*(np.pi/180.0))
Xd = np.empty((n_frames,2*dih_tot))
for i in range(n_frames):
    Xd[i] = np.vstack((cosv[i,:],sinv[i,:])).T.flatten()
```

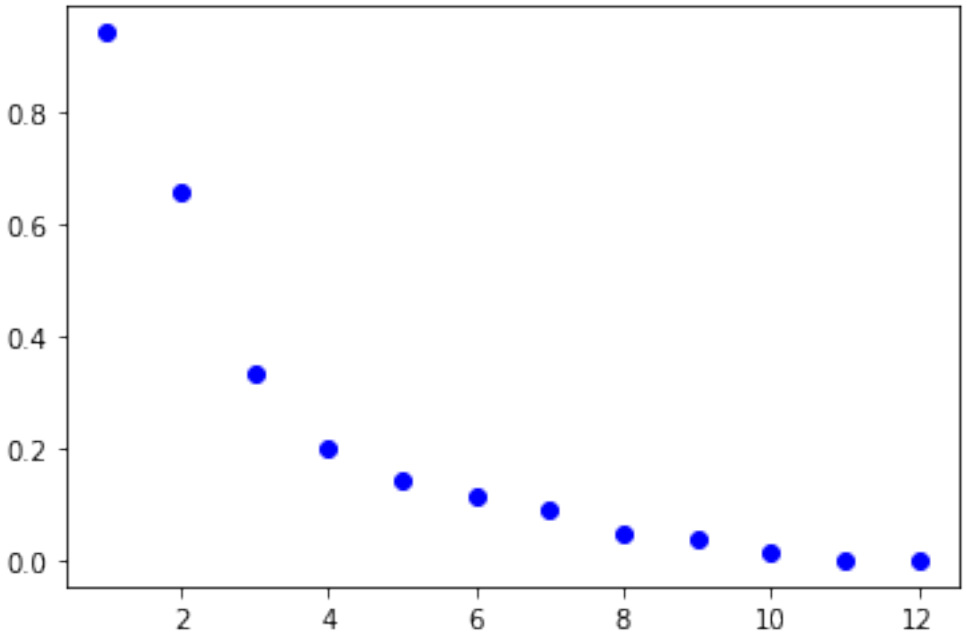
[22]:
```
pca = PCA(n_components=12)
proj = pca.fit_transform(Xd)
```

[23]:
```
print("DPCA eigenvalues and corresponding weight")
tot_var = 0
for i in range(len(pca.explained_variance_ratio_)):
    tot_var = tot_var +100*pca.explained_variance_ratio_[i]
    print("%10.6f  %10.6f  %10.6f" %(pca.explained_variance_[i],\
                                     100*pca.
 ↪explained_variance_ratio_[i],tot_var))
```

```
DPCA eigenvalues and corresponding weight
  0.940546   36.504586   36.504586
  0.655210   25.430073   61.934659
  0.331575   12.869124   74.803783
  0.200216    7.770809   82.574593
  0.141750    5.501606   88.076199
  0.112726    4.375151   92.451349
  0.088738    3.444107   95.895457
  0.050013    1.941114   97.836570
  0.037735    1.464561   99.301131
  0.015326    0.594846   99.895977
  0.001889    0.073317   99.969294
  0.000791    0.030706  100.000000
```

[24]:
```
plt.plot((np.linspace(1,12,num=12,dtype='int')),pca.explained_variance_,'bo')
```

[24]:
```
[<matplotlib.lines.Line2D at 0x7f148e5ac4c0>]
```



2.5 Kernel PCA

PCA assumes that a linear boundary can be drawn

2.5.1 Higher dimensionality projection

basic idea: project linearly inseparable data onto a higher dimensional space where it becomes linearly separable.

Suppose the decision boundary is described by a second order polynomial as above: $y^2 = r^2 + bx^2$. If we go to a higher dimensionality space in which the axes are x, x^2, y, the circle becomes a linear function and the decision boundary becomes a hyperplane.

Direct projection on the higher dimension space is computationally costly. We assume the projection can be done withs nonlinear mapping function $\mathbf{k}$ so that the mapping of a sample x can be written as $x \to \mathbf{k}(x)$. $\mathbf{k}$ is a *kernel function*.
The *Kernel* is the dot product of the images of the samples x under $\mathbf{k}$:

$$\mathbf{K}(\vec{x}_i, \vec{x}_j) = \mathbf{k}(\vec{x}_i)\mathbf{k}(\vec{x}_j)^T$$

where $\vec{x}_i \in R^d$, $\mathbf{k}(x_i) \in R^k$, $k > d$

$\mathbf{k}$ maps the original d features into k features which are nononlinear combinations of the original features. We assume that $\mathbf{K}$ yields the same result in the low dimension space.

Example:

$$x = (x_1, x_2, x_3)^T$$

$$f(x) = x^T x$$

$$f(x) = (x_1x_1, x_1x_2, x_1x_3, x_2x_1, x_2x_2, x_2x_3, x_3x_1, x_3x_2, x_3x_3)^T$$

Suppose $x_i = x_j = (1, 2, 3)$
Direct calculation in the high dimensional space is:

$f(x_i) * f(x_j)^T = [1, 2, 3, 2, 4, 6, 3, 6, 9][1, 2, 3, 2, 4, 6, 3, 6, 9]^T = 1+4+9+4+16+36+9+36+81 = 196$

But $f(x_i) * f(x_j)^T = K(x_i, x_j) = (x_j^T, x_i)^2$ hence:

$$K(x_i, x_j) = ([1, 2, 3]^T[1, 2, 3])^2 = 14^2 = 196$$

Not every projection to a higher space has an associated kernel function.

kernel methods is cheaper than direct projection but still intesive: you need the R^{NxN} kernel matrix

2.5.2 Gaussian kernel

One commonly used kernel is Gaussian Radial Basis Function (RBF) one:

$$\mathbf{K}(x_i, x_j) = exp(-\gamma||x_i - x_j||^2)$$

where $\gamma = \frac{1}{2\sigma^2}$ is a parameter.

2.5.3 KPCA step by step

PCA: we need to compute the complete variance-covariance matrix and diagonalize it:

$$C = \frac{1}{N}\sum_{i=1}^{N} \vec{x}_i \vec{x}_i^T$$

Kernel PCA: we would need to compute the covariance matrix in kernel space:

$$C = \frac{1}{N}\sum_{i=1}^{N} \mathbf{k}(\vec{x}_i)\mathbf{k}(\vec{x}_i)^T$$

instead we compute the *Kernel* matrix:

$$K = \frac{1}{N}\sum_{i=1}^{N} \mathbf{K}(\vec{x}_i \vec{x}_i^T)$$

for a gaussian kernel:

$$K_{ij} = exp(-\gamma||\vec{x}_i - \vec{x}_j||^2)$$

we do not obtain the principal components bu rather their *projections*

Since it is not guaranteed that the kernel matrix is centered, we can apply the following equation to do so:

$$K' = K - \mathbf{1}_N K - K\mathbf{1}_N + \mathbf{1}_N K \mathbf{1}_N$$

[25]:
```
class simple_kpca:
    """
    Simple class for kernel PCA vaguely mimicking Sklearn API
    """
    def __init__(self,n_components, kernel="rbf"):
        """
        create an estimator of n components and choose kernel
        only rbf kernel currently supported
        """
        self.n_components = n_components
        if kernel != "rbf":
            raise NotImplemented
        else:
            self.kernel = "gaussian"

    def fit_transform(self, gamma, X):
        """
        Calculate Kernel matrix and diagonalize it
        Arguments: X: n points x m features input data set, gamma: 1/2 sigma^2
        """
        # squared distances, this is the argument of the kernel
        D2 = sp.spatial.distance.pdist(X, metric='sqeuclidean')
```

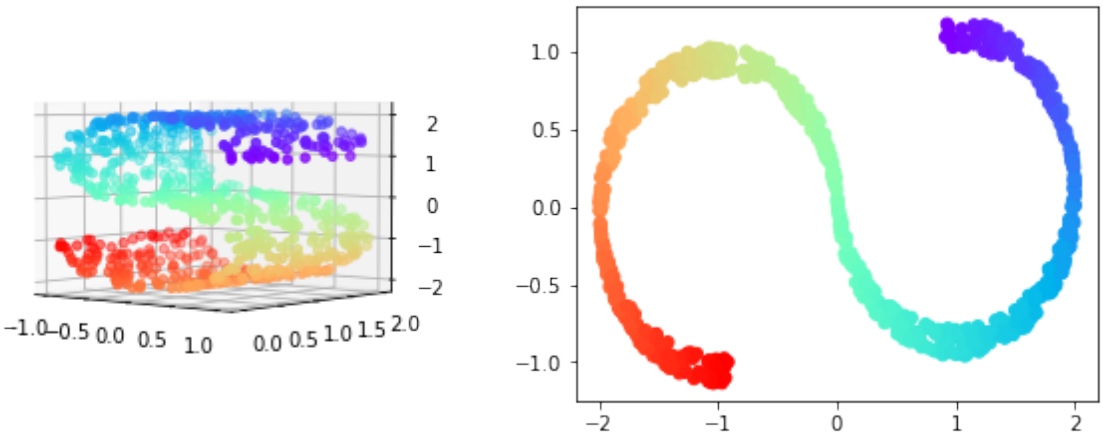
```
        D2 = sp.spatial.distance.squareform(D2)
        # compute K(x,xT)
        if self.kernel == "gaussian":
            K = np.exp(-gamma*D2)
        else:
            raise NotImplemented
        # apply centering
        N = K.shape[0]
        one_n = np.ones((N,N)) / N
        K = K - one_n.dot(K) - K.dot(one_n) + one_n.dot(K).dot(one_n)
        #solve eigenvalue problem; this are not "true" eigenvalues in k space
        #but rather their projections
        # eigenvalues in descending order
        eigvals, eigvectors = eigh(K)
        eigvals = eigvals[::-1]
        eigvectors = eigvectors.T[::-1][:self.n_components]
        #eigvectors = np.column_stack((eigvectors[:,-i] for i in range(1,self.
↪n_components+1)))
        return eigvectors.T
```

Swiss roll

[26]:
```
from sklearn import manifold, datasets

n_points = 800
swiss_roll, color = datasets.make_s_curve(n_points, random_state=123)
n_components = 2

# PCA
pca = PCA(n_components=2)
swiss_pca = pca.fit_transform(swiss_roll)
```

[49]:
```
fig = plt.figure(figsize=(16, 8))

ax = fig.add_subplot(231, projection="3d")
ax.scatter(swiss_roll[:, 0], swiss_roll[:, 1], swiss_roll[:, 2], c=color,␣
↪cmap=plt.cm.rainbow)
ax.view_init(3, -50)

ax = fig.add_subplot(232)
ax.scatter(swiss_pca[:, 0], swiss_pca[:, 1], c=color, cmap=plt.cm.rainbow)
```

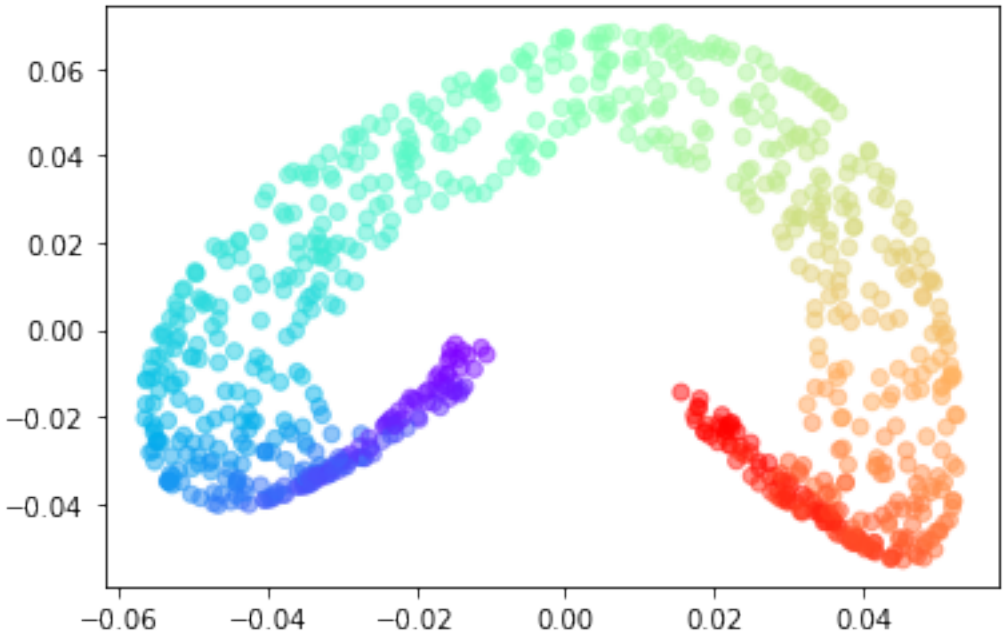
[49]:
```
<matplotlib.collections.PathCollection at 0x7f1477fde280>
```



[48]:
```
kpca = simple_kpca(n_components=2)
swiss_kpca = kpca.fit_transform(0.75, swiss_roll)
swiss_kpca = swiss_kpca
print(swiss_kpca.shape)
plt.scatter(swiss_kpca[:, 0], swiss_kpca[:, 1],  c=color,cmap=plt.cm.rainbow,␣
↪alpha=0.5)
```

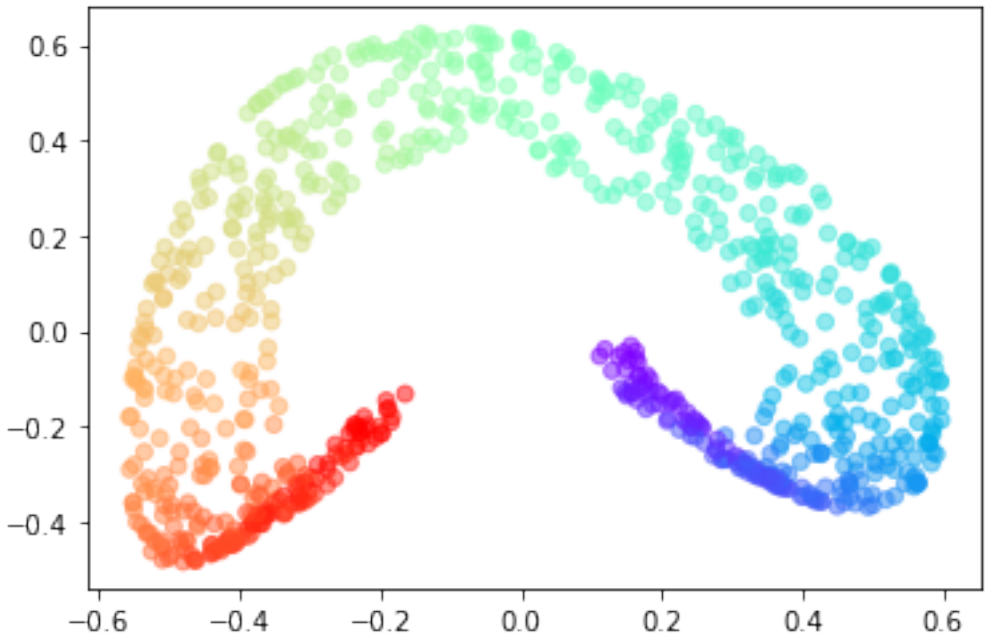
```
(800, 2)
```

[48]:
```
<matplotlib.collections.PathCollection at 0x7f14780ca3d0>
```



[47]:
```
from sklearn.decomposition import KernelPCA
scikit_kpca = KernelPCA(n_components=2, kernel='rbf', gamma=0.75)
swiss_sk_kpca = scikit_kpca.fit_transform(swiss_roll)
plt.scatter(swiss_sk_kpca[:, 0], swiss_sk_kpca[:, 1], c=color, cmap=plt.cm.
 ↪rainbow, alpha=0.5)
```

[47]:
```
<matplotlib.collections.PathCollection at 0x7f14782d5a90>
```



2.6 t-Distributed Stochastic Neighbor Embedding (tSNE)

t-SNE (Laurens van der Maatens and Geoffrey Hinton, Journal of Machine Learning Research 9(2008) 2579-2605)is an *unsupervised, non-linear* technique used to explore and visualize *high dimensional data.*

PCA seeks to maximize variance and pairwise distances hence objects that are *not near* in the complete space end up *far apart* in the reduced space. Not always the best for visualization (we may be interested in neighbourhood properties).

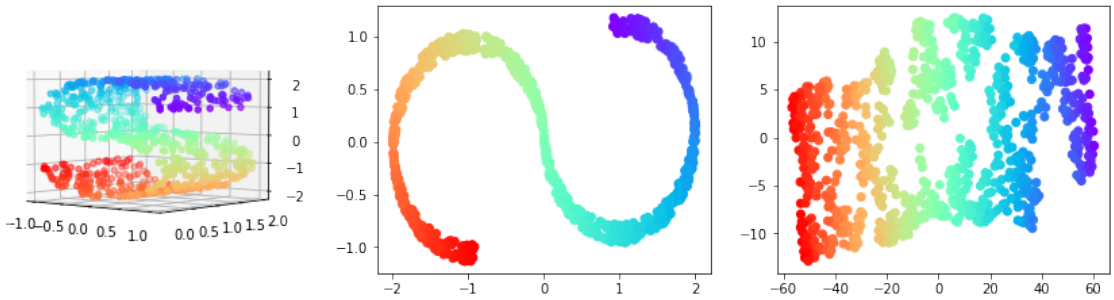
t-SNE preserves *only small pairwise distances* or *local similarities.* Example from the original paper:

[30]:
```
#tSNE
tsne = manifold.TSNE(n_components=2, init="pca", random_state=0)
swiss_tsne = tsne.fit_transform(swiss_roll)
```

[46]:
```
fig = plt.figure(figsize=(15, 8))
```

```
ax = fig.add_subplot(231, projection="3d")
ax.scatter(swiss_roll[:, 0], swiss_roll[:, 1], swiss_roll[:, 2], c=color,␣
↪cmap=plt.cm.rainbow)
ax.view_init(3, -50)

ax = fig.add_subplot(232)
ax.scatter(swiss_pca[:, 0], swiss_pca[:, 1], c=color, cmap=plt.cm.rainbow)

ax = fig.add_subplot(233)
ax.scatter(swiss_tsne[:, 0], swiss_tsne[:, 1], c=color, cmap=plt.cm.rainbow)
```

[46]: <matplotlib.collections.PathCollection at 0x7f1478175940>



Distance: > tSNE starts by calculating the probability of similarity of points in high-dimensional in the corresponding low-dimensional space. Similarity is calculated as the conditional probability x_i would choose x_j as its neighbour if the underlying distribution is a Normal centered in x_i

Minimization > It minimizes the difference between these conditional probabilities in higher-dimensional and lower-dimensional space for a perfect representation of data points in lower-dimensional space. To measure the minimization of the sum of difference of conditional probability t-SNE minimizes the sum of **Kullback-Leibler divergence** of overall data points using a gradient descent method.

KL divergence is a measure of how one probability distribution diverges from a second, expected probability distribution

Original input features *are no longer identifiable*, you *cannot* build back a reconstructed data set. Is mainly for **visualization**.

The join probability distribution in the hgh dimensional space is:

$$x_{ij} = \frac{x_{i|j} + x_{j|i}}{2n}$$

where

$$x_{j|i} = \frac{exp(-||x_j - x_i||^2)/2\sigma_i^2}{\sum_{k \neq j} exp(-||x_k - x_j||^2)/2\sigma_i^2}$$

The name ``t Distributed'' comes form the fact the distribution in the embedded space is:

$$xe_{ij} = \frac{1 + ||xe_j - xe_i||^2)}{\sum_{k \neq j} 1 + ||xe_k - xe_j||^2)}$$

and the cost to minimize is:

$$KL(P_{full}, P_{emb}) = \sum_{i \neq j} x_{ij} \frac{xe_{ij}}{x_{ij}}$$

tSNE advantages: - effective for embedding large dimensionality in 2D or 3D - does not accumulate points in the center from high dimensional data (as PCA does)

tSNE weaknesses: - computationally expensive, involves minimizing a cost function - stochastic: multiple runs starts with different seeds yield different results (also conbined with minimization) However, it is perfectly legitimate to pick the embedding with the least error.

2.7 Exercise

The file asp_LH_test.data.xz contains a Section ?? which includes the results of a Potential Energy Surface of aspartic acid in gas phase carried out with EAs (see Section ??.

The data set is accessed in this way

[32]:
```
import pandas as pd
asp_pes = pd.read_pickle("asp_LH_test.data.xz")
asp_pes.head()
```

[32]:

	(0, 3)	(3, 12)	(12, 14)	(3, 5)	(5, 8)	(8, 10)	\
0	-36.464000	14.538004	-176.916996	174.520995	-9.233997	179.186007	
1	-64.394064	-19.277872	-29.992921	171.892692	-169.747760	96.582077	
2	154.179123	168.436125	-125.606716	-72.657355	-43.874405	-171.043016	
3	-107.334178	-40.115131	-144.561949	-153.707466	55.440619	31.059754	
4	-132.371479	115.018847	90.234775	78.648060	-103.053836	-169.184848	

	energy	filename
0	-31.327645	asp_LH_test_00001.out.bz2
1	-31.277546	asp_LH_test_00002.out.bz2
2	-31.305746	asp_LH_test_00003.out.bz2
3	-31.288911	asp_LH_test_00004.out.bz2
4	-31.298300	asp_LH_test_00005.out.bz2

You can get a numpy array of dihedrals and energy in this way:

[33]:
```
RB = [(0, 3), (3, 12), (12, 14), (3, 5), (5, 8), (8, 10)]
dih = asp_pes[RB].to_numpy(dtype=float)
dih.shape
```

[33]: (4112, 6)

[34]:
```
EN = asp_pes['energy']
EN.shape
```

[34]: (4112,)

[35]:
```
Elow = EN[EN <= -31.3]
Elow
```

[35]:
```
0      -31.327645
2      -31.305746
16     -31.313200
18     -31.301481
24     -31.303836
          …
4107   -31.327470
4108   -31.321409
4109   -31.315854
4110   -31.329286
4111   -31.326718
Name: energy, Length: 4008, dtype: object
```

What you have to do: - convert energy from hartree to kJ/mol and calculate $\Delta E$with respect to the absolute minimum. See Section ?? - convert dihedrals in order to run DPCA and tSNE - graphs results correlating the projected space to the energy - which distance would you use to compare two points? - are all points relevant?

2.7.1 Solution

[36]:
```
har2kjmol = sp.constants.physical_constants["Avogadro constant"][0]\
*sp.constants.physical_constants["Hartree energy"][0]/1000.
print(har2kjmol)
gem = np.argmin(asp_pes['energy'])
deltaE = har2kjmol*(EN - EN[gem])
```

2625.4996394798254

We can discard structures with zero weight:

[37]:
```
deltaEF = deltaE[deltaE <= 30.].to_numpy(dtype=float)
deltaEF
```

[37]:
```
array([13.08030945, 10.10296292, 14.37034771, …, 29.45272538,
        8.77065567, 15.51237249])
```

[38]:
```
dih = asp_pes[RB]
dihF = dih[deltaE <= 30.].to_numpy(dtype=float)
```

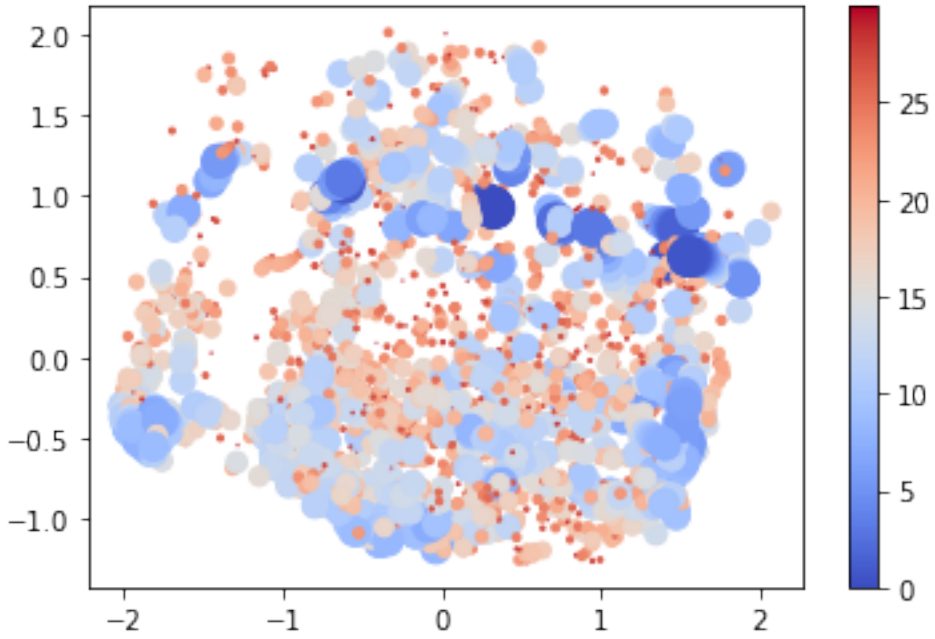
[39]:
```
deg2rad = np.pi/180.
s = np.sin(dihF*deg2rad)
c = np.cos(dihF*deg2rad)
v   = np.empty((dihF.shape[0], 2*dihF.shape[1]))
for i in range(dihF.shape[0]):
    v[i] = np.vstack((c[i,:],s[i,:])).T.flatten()
```

[40]:
```
pca = PCA(n_components = 6)
dpca = pca.fit_transform(v)
print("DPCA eigenvalues and corresponding weight")
tot_var = 0
for i in range(len(pca.explained_variance_ratio_)):
    tot_var = tot_var +100*pca.explained_variance_ratio_[i]
    print("%10.6f  %10.6f  %10.6f" %(pca.explained_variance_[i],\
                                          100*pca.
 ↪explained_variance_ratio_[i],tot_var))
```

```
DPCA eigenvalues and corresponding weight
  0.899295   22.132174   22.132174
  0.562832   13.851637   35.983811
  0.465273   11.450648   47.434459
  0.434622   10.696303   58.130763
  0.396001    9.745824   67.876587
  0.342578    8.431048   76.307635
```

[41]:
```
plt.scatter(dpca[:,0], dpca[:,1],c=deltaEF,cmap='coolwarm',s=(30.-deltaEF)**2/4)
plt.colorbar()
```

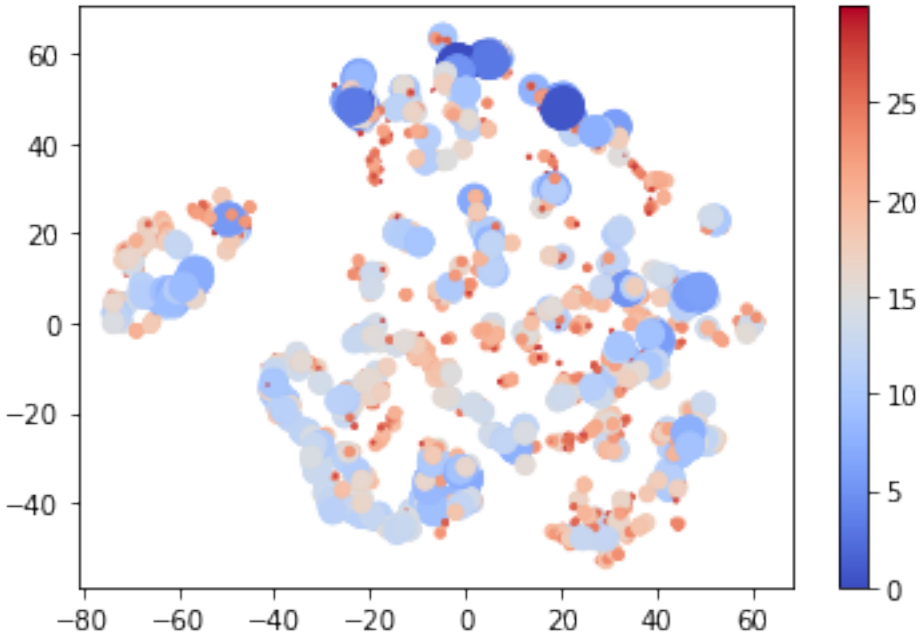
[41]:
```
<matplotlib.colorbar.Colorbar at 0x7f1478340d90>
```



[42]:
```
tsne = manifold.TSNE(n_components=2, init='pca')
tsne_results = tsne.fit_transform(v)
```

[43]:
```
plt.scatter(tsne_results[:,0], tsne_results[:
 ↪,1],c=deltaEF,cmap='coolwarm',s=(30-deltaEF)**2/4)
plt.colorbar()
```

[43]:
```
<matplotlib.colorbar.Colorbar at 0x7f14782f02b0>
```



2.8 Other techniques

- `Isomap`
- `Local Linear Embedding (LLE)`
- `Time Independent Component Analysis (TICA)`
- `Multidimensional Scaling (MDS)`

2.9 The End!