Principal Component Analysis ¶

The purpose of this notebook is to give an orientation of the salient features of PCA and how to access them.

In [1]:

```
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
pd.set_option('display.max_rows', 20)   # pandas: only print out 20 rows rather than the d
np.set_printoptions(precision=2, suppress=True)  # numpy: only print the first 2 decimal p
```

Load and view the data

We will use the bikes dataset we've discussed in class. Load in the data with the following command, inspect the columns, and visualise using a pairplot.

In [8]:

```
X = pd.read_csv("data/bikes.csv")
X
```

Out[8]:

	date	temperature	humidity	windspeed	count
0	2011-01-03	2.716070	45.715346	21.414957	120.000000
1	2011-01-04	2.896673	54.267219	15.136882	108.000000
2	2011-01-05	4.235654	45.697702	17.034578	82.000000
3	2011-01-06	3.112643	50.237349	10.091568	88.000000
4	2011-01-07	2.723918	49.144928	15.738204	148.000000
5	2011-01-08	1.967445	48.851252	17.035029	112.333333
6	2011-01-09	1.210973	48.557576	18.331855	76.666667
7	2011-01-10	0.454501	48.263900	19.628680	41.000000
8	2011-01-11	1.361393	59.623460	12.414597	43.000000
9	2011-01-12	1.541997	54.775880	25.432188	25.000000
...	...	...	...	...	...
719	2012-12-22	7.609421	56.748790	23.342550	205.333333
720	2012-12-23	6.030497	61.115812	16.277130	189.666667
721	2012-12-24	4.451573	65.482835	9.211711	174.000000
722	2012-12-25	4.750319	66.377012	17.747048	91.500000
723	2012-12-26	5.049065	67.271190	26.282385	9.000000
724	2012-12-27	5.587201	57.755931	28.678187	247.000000
725	2012-12-28	5.545775	54.242931	14.792709	644.000000
726	2012-12-29	4.924888	54.010283	14.777848	575.666667
727	2012-12-30	4.304001	53.777635	14.762987	507.333333
728	2012-12-31	3.683114	53.544987	14.748127	439.000000

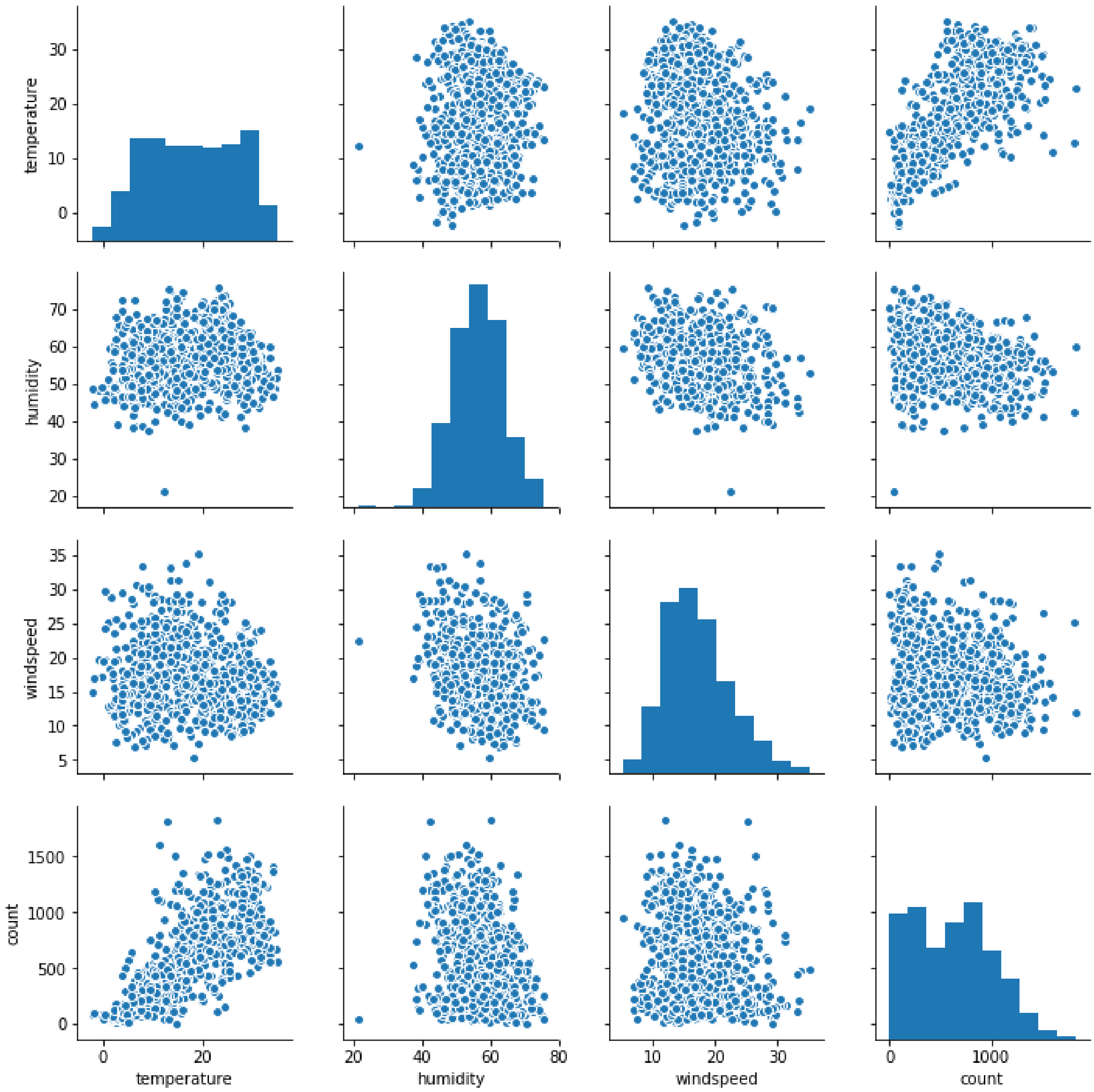
729 rows × 5 columns

In [9]:

```
sns.pairplot(X)    #pairplot is good but if you have too many columns it is not so good, e
```

Out[9]:

<seaborn.axisgrid.PairGrid at 0x18ad56ade48>

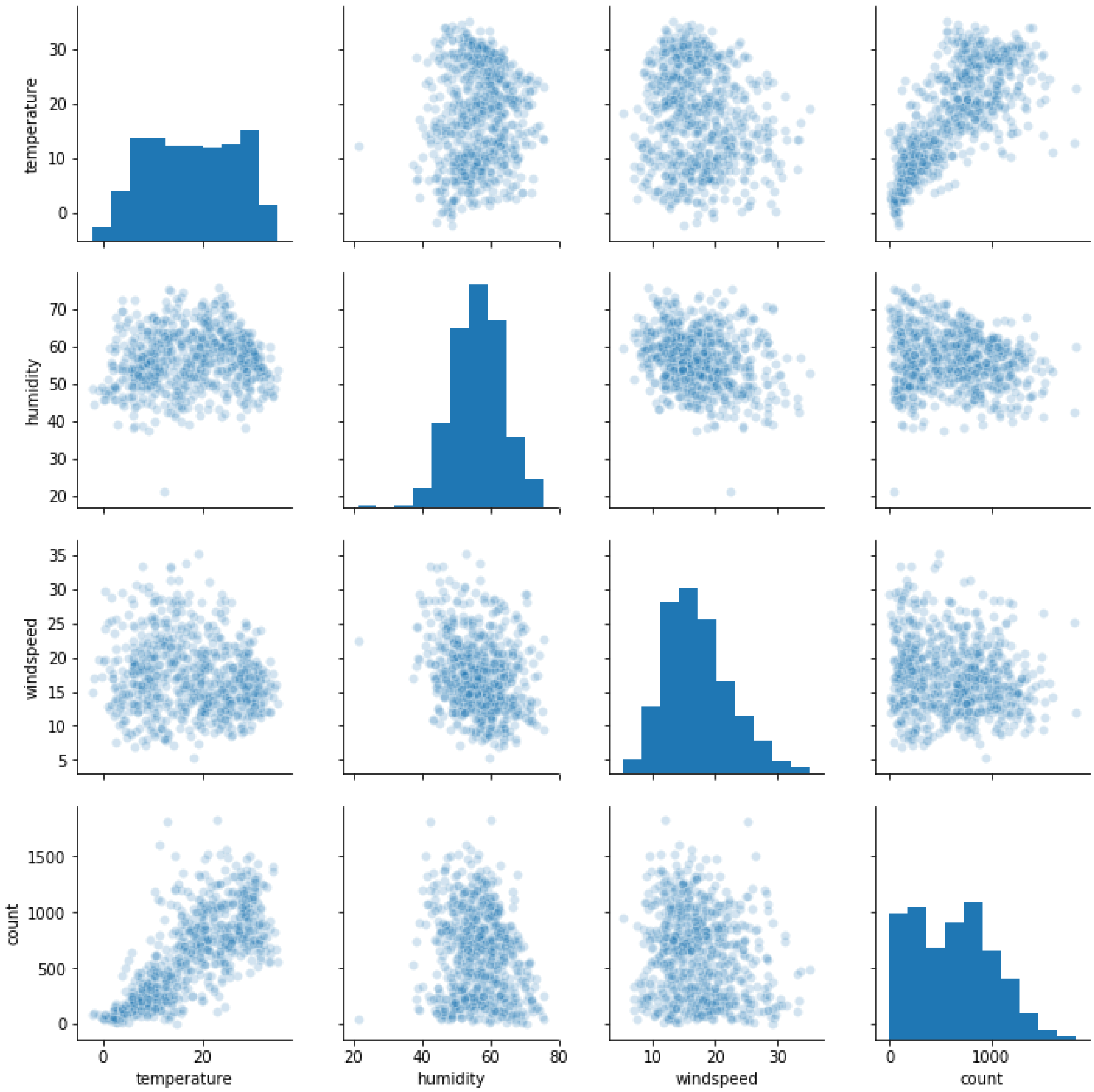


In [15]:

```
sns.pairplot(X, plot_kws=dict(alpha = 0.2))   #gives us an idea of the density of our plot.
```

Out[15]:

```
<seaborn.axisgrid.PairGrid at 0x18ad7f727b8>
```



Scikit-learn's PCA

The sklearn PCA model follows the same workflow as before:

- Instantiate the object
- Fit the object using the `.fit(...)` command.

Fitting the model

Have a look at the docs to see what Parameters are available to you. Crucially,

- Which transformations did we say are needed before performing PCA? the transformation we talked about were removing the mean and standardising the variants.

- Does sklearn's PCA do these for you?

Before fitting the model, perform/consider the following transformations of the raw data:

- Remove the date column. [Bonus question:] Is there some transformation that would make sense to keep in here?
- Should you make each column unit variance? (That is, `X.std(0) == zeros(d)` ?)

So, ensuring that the data matrix is suitably transformed (if neccessary), instantiate a PCA object. Make sure you do not specify the number of components: we want to return all principal components. Then fit the model to your transformed data.

In [17]:

```
from sklearn.decomposition import PCA
```

In [19]:

```
X_tform = X.drop('date', axis=1)
X_tform /= X_tform.std(0)
```

In [20]:

```
pca = PCA()
```

In [21]:

```
pca.fit(X_tform)
```

Out[21]:

```
PCA(copy=True, iterated_power='auto', n_components=None, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)
```

In [23]:

```
pca.components_
```

Out[23]:

```
array([[-0.68, -0.04,  0.27, -0.68],
       [ 0.06, -0.76,  0.61,  0.23],
       [ 0.3 ,  0.6 ,  0.74, -0.04],
       [-0.67,  0.25,  0.11,  0.7 ]])
```

Investigating the fitted model

If you have standardised your columns, your principal component matrix W should look as follows:

-0.68	-0.04	0.27	-0.68
0.06	-0.76	0.61	0.23
0.30	0.60	0.74	-0.04
-0.67	0.25	0.11	0.70

Obtaining the values of W and A for your fitted model is easy.

To retrieve the matrix W calculated by the model use:

- `.components_`

To retrieve the new co-ordinates, the matrix A, use:

- `.fit_transform([your data])`

In [24]:

```
W = pca.components_
A = pca.fit_transform(X_tform)
```

Interpreting PCA

- What does the first row of the matrix W mean?
- Is it significant that most of the values are negative?

In [ ]:

```
# The first row is the first principal component, i.e. the direction of greatest variance
# through the dataset. Recall that the data in our case was standardised such that all
# columns have unit variance. If one were able to plot the data in 4D space, it is this
# direction that would exhibit the largest 'stretch'.
#
# The direction itself is indicative that temperature and bike count correspond to the mos
# substantial correlation and variation in the dataset, and that this relationship is wort
# exploring.
#
# The sign of the direction is arbitrary, i.e. we can multiply all elements by -1, and the
# vector still describes the same subspace (it would simply flip the space over 180 degree
# However, it is significant that the 'windspeed' factor is of the opposite sign, meaning
# that this relationship is even stronger if including windspeed, but if we travel along
# *increasing* temperature, then this relationship involves *reducing* windspeed.
#
# If anything, this unsupervised analysis is indicative that performing regression on
# Bike Count is a sensible idea.
#
```

Explained Variance

Calculate the covariance of the new coordinates constructed by PCA.

- What is the correlation between each dimension of this new basis?
- How much variation is contained within each subspace?
- Now find the "explained variance" calculated by sklearn. This is the attribute: `.explained_variance_` .
- What is the relationship here?
- Calculate the cumulative `.explained_variance_ratio_` (hint: use `np.cumsum`). What do you think this view might be useful for?

In [26]:

```
np.corrcoef(A.T)
```

Out[26]:

```
array([[ 1.,  0.,  0., -0.],
       [ 0.,  1., -0., -0.],
       [ 0., -0.,  1.,  0.],
       [-0., -0.,  0.,  1.]])
```

In [27]:

```
np.var(A, axis=0)
```

Out[27]:

```
array([1.8 , 1.24, 0.75, 0.21])
```

In [28]:

```
pca.explained_variance_    #explained variance is how much variance exists in each princip
```

Out[28]:

```
array([1.8 , 1.24, 0.75, 0.21])
```

In [29]:

```
pca.explained_variance_ratio_  #The percentage of variance of the original data cloud can
                                #individual components
```

Out[29]:

```
array([0.45, 0.31, 0.19, 0.05])
```

In [30]:

```
pca.explained_variance_ / sum(pca.explained_variance_)
```

Out[30]:

```
array([0.45, 0.31, 0.19, 0.05])
```

In [31]:

```
np.cumsum(pca.explained_variance_ratio_)
```

Out[31]:

```
array([0.45, 0.76, 0.95, 1.  ])
```

Visualise the subspaces

Plot the principal 2D subspace, i.e. the 2D subspace that captures the most variation.

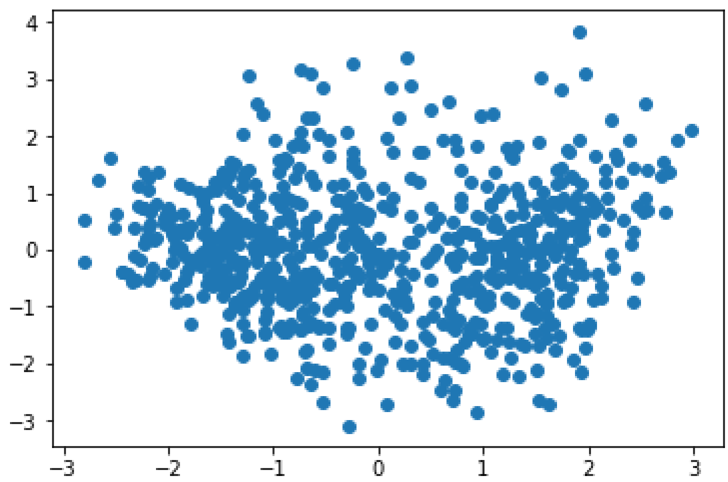
- How much variation of the original dataset has this captured?
- To what extent can we trust this plot as a valid representation of our data?
- By providing an interpretation of the second principal component, explain what this plot indicates about the original dataset.

In [32]:

```
plt.scatter(A[:,0], A[:,1]) #plot the first and second columns of A
# PC2 suggests that windspeed and humidity are anti-correlated in the original dataset.
# It also suggests that bike rental sales are also correlated with an increase of wind
# provided humidity decreases far enough. The fact that the former two are anti-correlated
# probably has more to do with the time of year than anything, and this might indicate
# the correlation with bike sales is not causal.
#
# There's not too much to say from the plot of the 2D subspace. At a push you can talk
# about the absence of datapoints in the negative quadrant, but by-and-large the
# data are well-spread within this subspace.
#
# The most notable feature is the possible presence of two clusters corresponding to
# low temperature and low sales, and high temperature and high sales. Again this may
# be more due to time of year than anything else.
```

Out[32]:

```
<matplotlib.collections.PathCollection at 0x18ad9e89b70>
```



In [39]:

```
#com add your code here to load the libraries and the data
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

data = pd.read_csv("data/companies_data.dat", header=None)
data.head()
```

Out[39]:

	0	1	2	3	4	5	6	7	8	9	...
0	0.20055	0.37951	0.39641	2.0472	32.351	0.38825	0.24976	1.3305	1.1389	0.50494	...
1	0.20912	0.49988	0.47225	1.9447	14.786	0	0.25834	0.99601	1.6996	0.49788	...
2	0.24866	0.69592	0.26713	1.5548	-1.1523	0	0.30906	0.43695	1.309	0.30408	...
3	0.081483	0.30734	0.45879	2.4928	51.952	0.14988	0.092704	1.8661	1.0571	0.57353	...
4	0.18732	0.61323	0.2296	1.4063	-7.3128	0.18732	0.18732	0.6307	1.1559	0.38677	...

5 rows × 65 columns

Cleaning and scaling the data

Even though this is not the key aim of this notebook, you still need to clean up the data (good practice!). In this case, it contains a few question marks that need to be removed.

- using `data.replace`, replace the `?` by `np.NaN`
- make sure the data types are right (check `data.dtypes`), if not apply `pd.to_numeric`
- drop the missing values with `dropna()`

Then

- import the `StandardScaler` from `sklearn` and apply it on the data, check that every feature is now centered and has unit variance

In [ ]:

```

```

[Bonus] Now have a go on a larger dataset

Sklearn houses a bunch of classic data science datasets. Let's use the Boston Housing data. Have a look at https://www.cs.toronto.edu/~delve/data/boston/bostonDetail.html (https://www.cs.toronto.edu/~delve/data/boston/bostonDetail.html) for more details. This is a much higher dimensinoal dataset, and can only really be explored by looking at various subspaces. Have a go at using PCA to learn about its features.

In [5]:

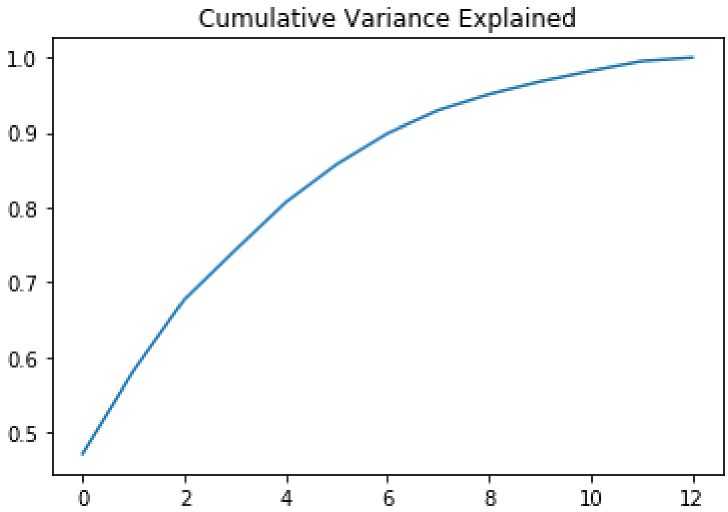
```
from sklearn import datasets
```

In [6]:

```
x, _ = datasets.load_boston(return_X_y=True)
```

In [37]:

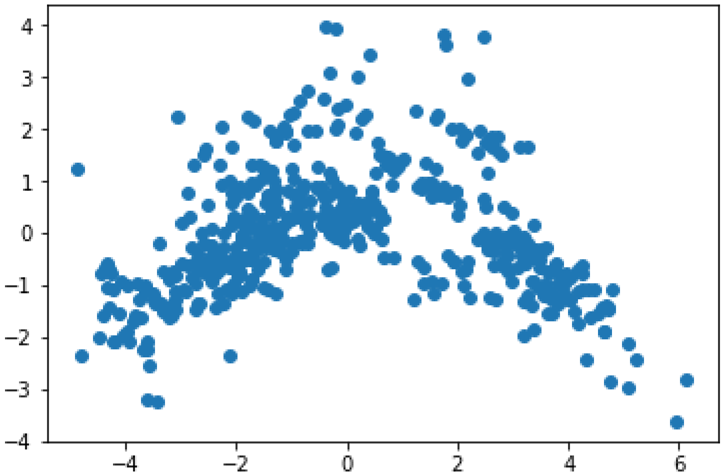
```
pca = PCA().fit(x / x.std(0))
W = pca.components_
A = pca.fit_transform(x / x.std(0))
plt.plot(np.cumsum(pca.explained_variance_ratio_))
plt.gca().set_title("Cumulative Variance Explained");
```



In [38]:

```
print(W)
plt.scatter(A[:,0], A[:,1]);
# The PCs here are quite dense, in that a lot of dimensions in the original
# dataset have a reasonable-sized contribution in terms of coefficients.
# Using the Toronto webpage, have a look to see if these make some kind
# of sense.
```

```
[[ 0.25 -0.26  0.35  0.01  0.34 -0.19  0.31 -0.32  0.32  0.34  0.2  -0.2
   0.31]
 [-0.32 -0.32  0.11  0.45  0.22  0.15  0.31 -0.35 -0.27 -0.24 -0.31  0.24
  -0.07]
 [ 0.25  0.3  -0.02  0.29  0.12  0.59 -0.02 -0.05  0.29  0.22 -0.32 -0.3
  -0.27]
 [ 0.06  0.13  0.02  0.82 -0.13 -0.28 -0.18  0.22  0.13  0.1   0.28  0.17
   0.07]
 [ 0.08  0.32 -0.01  0.09  0.14 -0.42  0.02  0.1  -0.2  -0.13 -0.58 -0.35
   0.39]
 [-0.22 -0.32 -0.08  0.17 -0.15  0.06 -0.07  0.02 -0.14 -0.19  0.27 -0.8
  -0.05]
 [ 0.78 -0.27 -0.34  0.07 -0.2   0.06  0.12 -0.1  -0.14 -0.31  0.    0.07
   0.09]
 [ 0.15 -0.4   0.17 -0.02  0.08 -0.33 -0.6  -0.12  0.08  0.08 -0.32 -0.
  -0.42]
 [ 0.26  0.36  0.64 -0.01 -0.02  0.05 -0.07 -0.15 -0.47 -0.18  0.25 -0.04
  -0.2 ]
 [ 0.02  0.27 -0.36 -0.01  0.23 -0.43  0.36 -0.17  0.02 -0.04  0.15 -0.1
  -0.6 ]
 [-0.11  0.26 -0.3   0.01  0.11  0.05 -0.46 -0.7   0.04 -0.1   0.17  0.02
   0.27]
 [ 0.09 -0.07 -0.11 -0.    0.8   0.15 -0.21  0.39 -0.11 -0.22  0.21  0.04
   0.06]
 [ 0.05 -0.08 -0.25  0.04  0.04  0.05 -0.04 -0.02 -0.63  0.72  0.02 -0.
   0.02]]
```



In [ ]: