

# Download data

Data available via scikit-learn

<https://scikit-learn.org/stable/modules/classes.html#module-sklearn.datasets> (<https://scikit-learn.org/stable/modules/classes.html#module-sklearn.datasets>)

<https://towardsdatascience.com/understanding-k-means-clustering-in-machine-learning-6a6e67336aa1>  
(<https://towardsdatascience.com/understanding-k-means-clustering-in-machine-learning-6a6e67336aa1>)

```

In [1]: %matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
##### clustering (unsupervised/descrete) #####
# random generated data
# Generating 3 distinct cluster, 2 of them slightly overlapping
X = -2 * np.random.rand(50,2)
X1 = 1 + 2 * np.random.rand(50,2)
X2 = 0.4 + np.random.rand(50,2)

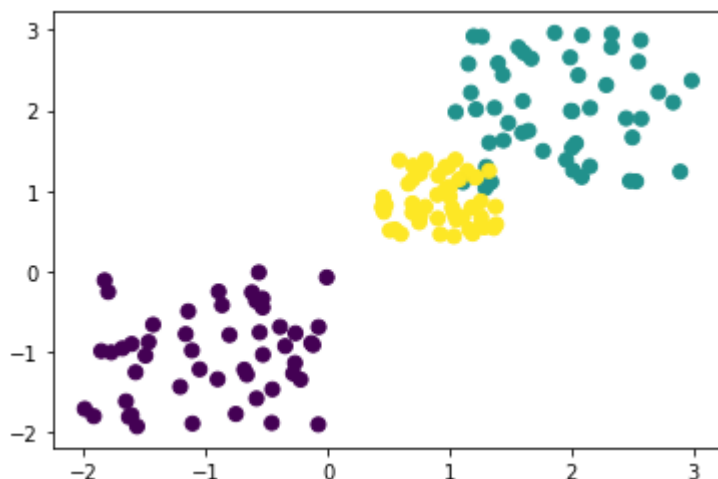
X = np.append(X,X1,axis=0)
X = np.append(X,X2,axis=0)
colors = [0]*50+[1]*50+[2]*50
# === PLOTTING DATA
print(X.shape)
plt.scatter(X[ : , 0], X[ :, 1], s = 50, c = colors)
plt.show()
# ===

# gene expression
nci60 = pd.read_csv('data/NCI60.txt',sep='\t', index_col=False)
# print(nci60.shape)
# display(nci60)
### pre-process
print(nci60.shape)
# expression data starts at column 5
expr = nci60.iloc[:,5:]
print(expr.shape)

##### dimensionality reduction (unsupervised/continuous) #####
#https://idyll.pub/post/dimensionality-reduction-293e465c2a3443e8941b016d/
#gene expression

```

(150, 2)



(198, 389)

(198, 384)

# K-Means

## K-means synthenic data

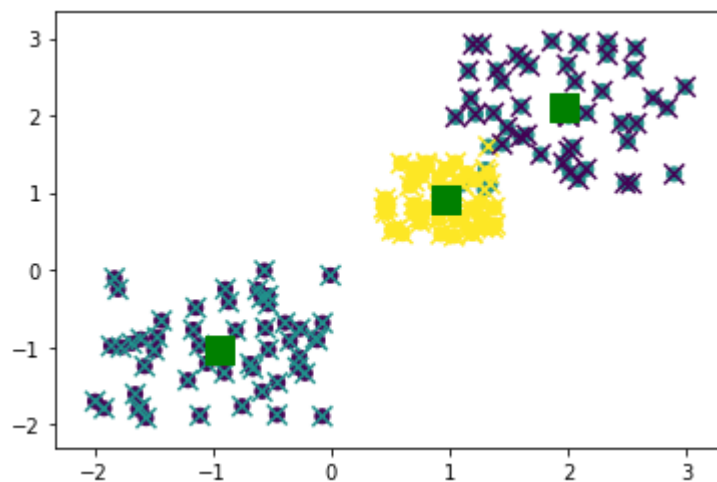
```
In [2]: #Synthetic data
from sklearn.cluster import KMeans
Kmean = KMeans(n_clusters=3)
Kmean.fit(X)

print(Kmean.cluster_centers_)

# Plots original points
plt.scatter(X[ : , 0], X[ : , 1], s = 50, c=colors)
# Plots X Labels after k-mens
plt.scatter(X[ : , 0], X[ : , 1], s = 100, marker='x', c=Kmean.labels_)

# Plots centroids
for cl in Kmean.cluster_centers_:
    plt.scatter(cl[0], cl[1], s=200, c='g', marker='s')
plt.show()
```

```
[[ 1.95967537  2.10576763]
 [-0.93685732 -1.02268501]
 [ 0.97224279  0.90732231]]
```



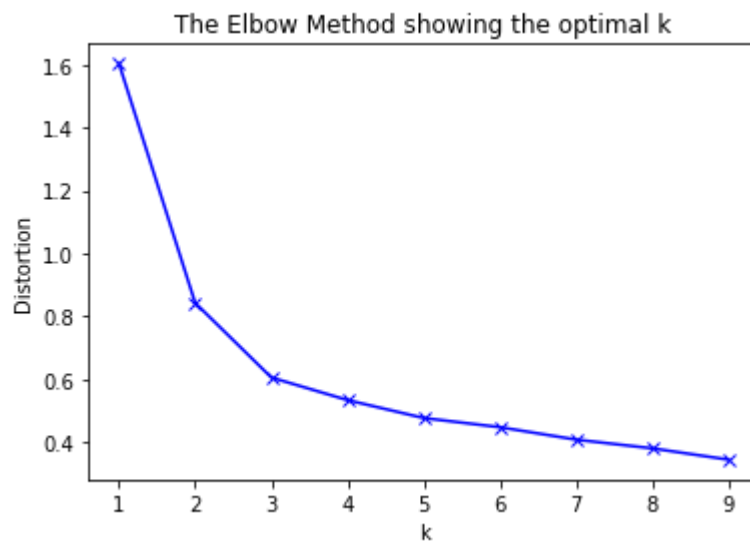
## Elbow method for determing K

<https://pythonprogramminglanguage.com/kmeans-elbow-method/>  
[\(https://pythonprogramminglanguage.com/kmeans-elbow-method/\)](https://pythonprogramminglanguage.com/kmeans-elbow-method/)

```
In [3]: from scipy.spatial.distance import cdist

# k means determine k
distortions = []
K = range(1,10)
for k in K:
    kmeanModel = KMeans(n_clusters=k).fit(X)
    kmeanModel.fit(X)
    # calculates the distance between each point and each cluster center
    # takes the minimum of each calculation (hence the difference between point and ITS cluster center)
    # takes average of all distances
    distortions.append(sum(np.min(cdist(X, kmeanModel.cluster_centers_, 'euclidean'), axis=1)) / X.shape[0])

# Plot the elbow
plt.plot(K, distortions, 'bx-')
plt.xlabel('k')
plt.ylabel('Distortion')
plt.title('The Elbow Method showing the optimal k')
plt.show()
```



## K-means on Gene Expression data

```
In [4]: display(nci60)
display(expr)
# fit the data, there is 9 tissue types
Kmean = KMeans(n_clusters=16)
Kmean.fit(expr)
# see how many rows ended up with each labels
print(pd.Series(Kmean.labels_).value_counts())
print(nci60.batch.value_counts())

# # how we do visulaize this?

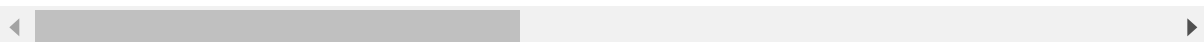
plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=Kmean.labels_)
plt.show()

plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=nci60.batch.astype('c
ategory').cat.codes)
plt.show()
```

|     | tissue    | batch           | PC1 | PC2       | PC3       | ACAD10    | ACOT9     | ACP5      |   |
|-----|-----------|-----------------|-----|-----------|-----------|-----------|-----------|-----------|---|
| 0   | GSM803615 | cancer_leukemia | 1   | -0.056842 | -0.044581 | -0.113268 | -0.225523 | -0.657666 | - |
| 1   | GSM803674 | cancer_leukemia | 1   | -0.056585 | -0.042994 | -0.114095 | -0.115336 | -0.745160 | - |
| 2   | GSM803733 | cancer_leukemia | 1   | -0.055702 | -0.045556 | -0.112062 | 0.061519  | 0.074016  | - |
| 3   | GSM803616 | cancer_leukemia | 1   | -0.061005 | -0.036062 | -0.123295 | -0.148417 | 0.195879  | - |
| 4   | GSM803675 | cancer_leukemia | 1   | -0.060836 | -0.032265 | -0.127681 | -0.198627 | 0.117102  | - |
| 5   | GSM803734 | cancer_leukemia | 1   | -0.056634 | -0.049184 | -0.128937 | -0.083067 | 0.694710  | - |
| 6   | GSM803617 | cancer_leukemia | 1   | -0.058637 | -0.027791 | -0.107388 | -0.154221 | 0.820919  | - |
| 7   | GSM803676 | cancer_leukemia | 1   | -0.058000 | -0.029718 | -0.105948 | -0.213438 | 0.862094  | - |
| 8   | GSM803735 | cancer_leukemia | 1   | -0.053656 | -0.054039 | -0.126916 | 0.104375  | 0.651555  | - |
| 9   | GSM803618 | cancer_leukemia | 1   | -0.061899 | -0.064274 | -0.104224 | -0.081437 | 0.827006  | - |
| 10  | GSM803677 | cancer_leukemia | 1   | -0.060902 | -0.064753 | -0.107330 | -0.183441 | 0.852921  | - |
| 11  | GSM803736 | cancer_leukemia | 1   | -0.062722 | -0.062989 | -0.100799 | -0.132196 | 1.089384  | - |
| 12  | GSM803619 | cancer_leukemia | 1   | -0.065582 | -0.017462 | -0.055630 | -0.237170 | 0.864546  | - |
| 13  | GSM803678 | cancer_leukemia | 1   | -0.064839 | -0.021478 | -0.060321 | -0.293436 | 0.878104  | - |
| 14  | GSM803737 | cancer_leukemia | 1   | -0.064517 | -0.018884 | -0.056781 | -0.224833 | 0.954050  | - |
| 15  | GSM803620 | cancer_leukemia | 1   | -0.067114 | -0.034380 | -0.089720 | -0.135940 | 0.892611  | - |
| 16  | GSM803679 | cancer_leukemia | 1   | -0.067142 | -0.034965 | -0.086943 | -0.139152 | 0.960512  | - |
| 17  | GSM803738 | cancer_leukemia | 1   | -0.066316 | -0.043587 | -0.095912 | -0.101752 | 1.026879  | - |
| 18  | GSM803621 | cancer_breast   | 1   | -0.078022 | 0.047675  | 0.067187  | -0.451185 | 0.940607  | - |
| 19  | GSM803680 | cancer_breast   | 1   | -0.077909 | 0.048376  | 0.065161  | -0.488317 | 0.976915  | - |
| 20  | GSM803739 | cancer_breast   | 1   | -0.078001 | 0.044726  | 0.064545  | -0.341475 | 1.100175  | - |
| 21  | GSM803622 | cancer_breast   | 1   | -0.076179 | 0.063242  | 0.091899  | -0.652644 | 0.618990  | - |
| 22  | GSM803681 | cancer_breast   | 1   | -0.076027 | 0.064693  | 0.091411  | -0.629674 | 0.598216  | - |
| 23  | GSM803740 | cancer_breast   | 1   | -0.075180 | 0.063560  | 0.094382  | -0.569921 | 0.655253  | - |
| 24  | GSM803623 | cancer_breast   | 1   | -0.072455 | -0.068390 | -0.088982 | -0.345481 | 0.251308  | - |
| 25  | GSM803682 | cancer_breast   | 1   | -0.072869 | -0.071157 | -0.084977 | -0.186985 | 0.359076  | - |
| 26  | GSM803741 | cancer_breast   | 1   | -0.072874 | -0.069472 | -0.087196 | -0.193552 | 0.421299  | - |
| 27  | GSM803624 | cancer_ovarian  | 1   | -0.077715 | 0.004067  | 0.010490  | -0.568091 | 0.616888  | - |
| 28  | GSM803683 | cancer_ovarian  | 1   | -0.080732 | 0.006610  | 0.028655  | -0.655521 | 0.658422  | - |
| 29  | GSM803742 | cancer_ovarian  | 1   | -0.080749 | 0.006198  | 0.029227  | -0.454352 | 0.804546  | - |
| ... | ...       | ...             | ... | ...       | ...       | ...       | ...       | ...       |   |
| 168 | GSM803672 | cancer_melanoma | 1   | -0.072058 | 0.019348  | 0.045163  | -0.340114 | 0.656020  |   |
| 169 | GSM803730 | cancer_melanoma | 1   | -0.073148 | 0.018081  | 0.040628  | -0.489069 | 0.747809  |   |
| 170 | GSM803787 | cancer_melanoma | 1   | -0.074256 | 0.023280  | 0.047394  | -0.375733 | 0.791462  |   |
| 171 | GSM803673 | cancer_breast   | 1   | -0.072343 | -0.060815 | -0.056714 | -0.212072 | 0.612341  | - |

|     | tissue    | batch           | PC1 | PC2       | PC3       | ACAD10    | ACOT9     | ACP5      |   |
|-----|-----------|-----------------|-----|-----------|-----------|-----------|-----------|-----------|---|
| 172 | GSM803731 | cancer_breast   | 1   | -0.072348 | -0.058145 | -0.057504 | -0.220204 | 0.639464  | - |
| 173 | GSM803788 | cancer_breast   | 1   | -0.072220 | -0.060890 | -0.058461 | -0.174758 | 0.691322  | - |
| 174 | GSM18933  | normal_brain    | 2   | -0.021123 | 0.201263  | -0.082889 | -0.333775 | -0.469165 | - |
| 175 | GSM18934  | normal_brain    | 2   | -0.020917 | 0.203883  | -0.088022 | -0.298711 | -0.389676 | - |
| 176 | GSM18923  | normal_brain    | 2   | -0.017381 | 0.198927  | -0.075512 | -0.174182 | -0.412700 | - |
| 177 | GSM18924  | normal_brain    | 2   | -0.017633 | 0.198388  | -0.081087 | -0.121340 | -0.431464 | - |
| 178 | GSM18929  | normal_brain    | 2   | -0.018627 | 0.211270  | -0.084287 | -0.388273 | -0.395204 | - |
| 179 | GSM18930  | normal_brain    | 2   | -0.022591 | 0.188253  | -0.072763 | -0.278641 | -0.470682 | - |
| 180 | GSM18917  | normal_brain    | 2   | -0.023064 | 0.193976  | -0.104031 | -0.397680 | -0.465619 | - |
| 181 | GSM18918  | normal_brain    | 2   | -0.022722 | 0.198841  | -0.098570 | -0.125040 | -0.515103 | - |
| 182 | GSM18997  | normal_ovary    | 2   | -0.013734 | 0.170145  | -0.110469 | 0.037138  | -0.304679 | - |
| 183 | GSM18998  | normal_ovary    | 2   | -0.013945 | 0.167311  | -0.109352 | -0.093727 | -0.316046 | - |
| 184 | GSM18957  | normal_prostate | 2   | -0.034817 | 0.150056  | -0.107471 | -0.517187 | -0.473539 | - |
| 185 | GSM18958  | normal_prostate | 2   | -0.033561 | 0.140488  | -0.114631 | -0.350905 | -0.402720 | - |
| 186 | GSM18889  | normal_blood    | 2   | -0.027525 | 0.126379  | -0.165823 | -0.263033 | -0.073894 | - |
| 187 | GSM18890  | normal_blood    | 2   | -0.028814 | 0.121179  | -0.166312 | -0.217535 | -0.127278 | - |
| 188 | GSM18877  | normal_blood    | 2   | -0.016501 | 0.113063  | -0.174482 | -0.011065 | -0.153146 | - |
| 189 | GSM18878  | normal_blood    | 2   | -0.016110 | 0.113215  | -0.176995 | -0.021145 | -0.136286 | - |
| 190 | GSM18875  | normal_blood    | 2   | -0.022206 | 0.108500  | -0.164317 | -0.182053 | -0.337838 | - |
| 191 | GSM18876  | normal_blood    | 2   | -0.019868 | 0.119745  | -0.167830 | -0.325988 | -0.284017 | - |
| 192 | GSM18949  | normal_lung     | 2   | -0.026617 | 0.161477  | -0.096402 | -0.422320 | -0.494245 |   |
| 193 | GSM18950  | normal_lung     | 2   | -0.022855 | 0.170397  | -0.100391 | -0.378157 | -0.352568 |   |
| 194 | GSM19001  | normal_skin     | 2   | -0.014454 | 0.172637  | -0.113487 | 0.444467  | -0.549839 | - |
| 195 | GSM19002  | normal_skin     | 2   | -0.014447 | 0.174409  | -0.117696 | 0.721574  | -0.511333 | - |
| 196 | GSM18955  | normal_kidney   | 2   | -0.030083 | 0.121079  | -0.114942 | -0.160365 | -0.533933 |   |
| 197 | GSM18956  | normal_kidney   | 2   | -0.029734 | 0.126442  | -0.114295 | -0.113225 | -0.417798 |   |

198 rows × 389 columns

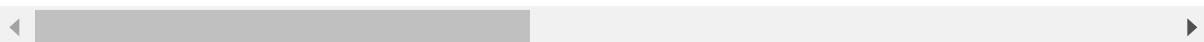


|     | ACAD10    | ACOT9     | ACP5      | ACSL3     | ACTN1    | ACTN4     | ACVR2A   | ADCK4     |       |
|-----|-----------|-----------|-----------|-----------|----------|-----------|----------|-----------|-------|
| 0   | -0.113268 | -0.225523 | -0.657666 | -0.719608 | 0.976008 | 1.111694  | 0.503365 | -0.544117 | -1.17 |
| 1   | -0.114095 | -0.115336 | -0.745160 | -0.694094 | 0.943915 | 1.002691  | 0.541647 | -0.107079 | -1.15 |
| 2   | -0.112062 | 0.061519  | 0.074016  | -0.465058 | 1.225343 | 0.800822  | 0.751530 | -0.304991 | -1.10 |
| 3   | -0.123295 | -0.148417 | 0.195879  | -0.766730 | 1.087944 | 1.520482  | 1.073094 | -0.145891 | -1.02 |
| 4   | -0.127681 | -0.198627 | 0.117102  | -0.464126 | 1.095090 | 1.549793  | 1.069821 | 0.029051  | -1.16 |
| 5   | -0.128937 | -0.083067 | 0.694710  | -0.342008 | 0.865687 | 1.393348  | 1.056934 | -0.321569 | -1.23 |
| 6   | -0.107388 | -0.154221 | 0.820919  | -0.552283 | 1.209606 | 1.006519  | 0.385098 | -0.079533 | -1.05 |
| 7   | -0.105948 | -0.213438 | 0.862094  | -0.628550 | 1.167257 | 1.036698  | 0.333438 | -0.449753 | -1.08 |
| 8   | -0.126916 | 0.104375  | 0.651555  | -0.419143 | 0.803217 | 1.201640  | 1.214298 | 0.505413  | -0.92 |
| 9   | -0.104224 | -0.081437 | 0.827006  | -0.493754 | 0.311060 | 0.098200  | 0.192633 | -0.071105 | -1.10 |
| 10  | -0.107330 | -0.183441 | 0.852921  | -0.470541 | 0.290231 | -0.026508 | 0.122113 | 0.041792  | -1.15 |
| 11  | -0.100799 | -0.132196 | 1.089384  | -0.307204 | 0.011621 | -0.278588 | 0.241486 | -0.426995 | -1.20 |
| 12  | -0.055630 | -0.237170 | 0.864546  | -0.840067 | 0.900479 | 1.689163  | 1.351323 | -0.071631 | -1.15 |
| 13  | -0.060321 | -0.293436 | 0.878104  | -0.863561 | 0.920503 | 1.672084  | 1.384987 | -0.059195 | -1.18 |
| 14  | -0.056781 | -0.224833 | 0.954050  | -0.845293 | 0.876780 | 1.488628  | 1.321521 | -0.125633 | -1.17 |
| 15  | -0.089720 | -0.135940 | 0.892611  | -0.600149 | 1.010743 | 1.150900  | 0.959611 | 0.286767  | -1.19 |
| 16  | -0.086943 | -0.139152 | 0.960512  | -0.392410 | 0.965920 | 1.242161  | 1.051196 | 0.258448  | -1.17 |
| 17  | -0.095912 | -0.101752 | 1.026879  | -0.437341 | 0.814904 | 0.986422  | 0.879281 | -0.173074 | -1.14 |
| 18  | 0.067187  | -0.451185 | 0.940607  | -0.984481 | 0.755387 | 1.609322  | 0.873873 | -0.225148 | -1.42 |
| 19  | 0.065161  | -0.488317 | 0.976915  | -0.925485 | 0.747708 | 1.592533  | 0.958221 | -0.238177 | -1.53 |
| 20  | 0.064545  | -0.341475 | 1.100175  | -0.898786 | 0.689580 | 1.450014  | 0.890532 | -0.462409 | -1.49 |
| 21  | 0.091899  | -0.652644 | 0.618990  | -0.868125 | 0.472090 | 1.679343  | 0.742354 | 0.162686  | -1.55 |
| 22  | 0.091411  | -0.629674 | 0.598216  | -0.941766 | 0.489222 | 1.749456  | 0.764734 | 0.128605  | -1.54 |
| 23  | 0.094382  | -0.569921 | 0.655253  | -0.793412 | 0.447984 | 1.574006  | 0.702518 | 0.077412  | -1.53 |
| 24  | -0.088982 | -0.345481 | 0.251308  | -0.751214 | 0.637299 | 1.005870  | 0.604459 | 0.118928  | -1.22 |
| 25  | -0.084977 | -0.186985 | 0.359076  | -0.810905 | 0.574677 | 1.093582  | 0.846591 | 0.107682  | -1.33 |
| 26  | -0.087196 | -0.193552 | 0.421299  | -0.793472 | 0.852449 | 0.861591  | 0.725070 | 0.059282  | -1.33 |
| 27  | 0.010490  | -0.568091 | 0.616888  | -1.029302 | 0.960891 | 1.780489  | 0.482121 | 0.290475  | -1.53 |
| 28  | 0.028655  | -0.655521 | 0.658422  | -0.864975 | 0.858157 | 1.999481  | 0.733460 | 0.219468  | -1.54 |
| 29  | 0.029227  | -0.454352 | 0.804546  | -0.732586 | 0.702438 | 1.773233  | 0.784342 | 0.139265  | -1.52 |
| ... | ...       | ...       | ...       | ...       | ...      | ...       | ...      | ...       | ...   |
| 168 | 0.045163  | -0.340114 | 0.656020  | 0.284666  | 1.160679 | 1.300248  | 0.765416 | -0.135345 | -1.55 |
| 169 | 0.040628  | -0.489069 | 0.747809  | 0.416655  | 1.144911 | 1.324996  | 0.843852 | -0.102116 | -1.49 |
| 170 | 0.047394  | -0.375733 | 0.791462  | 0.308832  | 1.202791 | 1.445058  | 1.075510 | -0.245130 | -1.52 |
| 171 | -0.056714 | -0.212072 | 0.612341  | -0.869982 | 0.143276 | 1.074310  | 0.387683 | -0.259083 | -1.29 |



|     | ACAD10    | ACOT9     | ACP5      | ACSL3     | ACTN1     | ACTN4     | ACVR2A    | ADCK4     |       |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-------|
| 172 | -0.057504 | -0.220204 | 0.639464  | -0.898149 | 0.210101  | 1.088200  | 0.397209  | -0.171641 | -1.30 |
| 173 | -0.058461 | -0.174758 | 0.691322  | -0.808267 | 0.128221  | 0.929756  | 0.411656  | -0.151958 | -1.40 |
| 174 | -0.082889 | -0.333775 | -0.469165 | -0.496119 | 0.318325  | -0.132482 | -0.085508 | -0.144946 | -0.49 |
| 175 | -0.088022 | -0.298711 | -0.389676 | -0.470748 | 0.364341  | -0.241940 | -0.065919 | -0.263852 | -0.49 |
| 176 | -0.075512 | -0.174182 | -0.412700 | -0.415713 | 0.222922  | -0.035956 | -0.012674 | -0.008977 | -0.40 |
| 177 | -0.081087 | -0.121340 | -0.431464 | -0.451556 | 0.295517  | -0.056207 | 0.129624  | -0.205905 | -0.41 |
| 178 | -0.084287 | -0.388273 | -0.395204 | -0.434761 | 0.571569  | 0.309640  | 0.185475  | -0.374542 | -0.49 |
| 179 | -0.072763 | -0.278641 | -0.470682 | -0.414257 | 0.503134  | 0.759271  | 0.424932  | -0.360431 | -0.48 |
| 180 | -0.104031 | -0.397680 | -0.465619 | -0.379339 | 0.083240  | -0.199214 | -0.274718 | -0.059897 | -0.46 |
| 181 | -0.098570 | -0.125040 | -0.515103 | -0.340250 | 0.227368  | -0.239526 | -0.158643 | -0.011989 | -0.52 |
| 182 | -0.110469 | 0.037138  | -0.304679 | -0.121934 | -0.175915 | 0.297356  | 0.196031  | -0.190083 | -0.35 |
| 183 | -0.109352 | -0.093727 | -0.316046 | -0.125807 | -0.098384 | 0.229316  | 0.235352  | -0.113389 | -0.33 |
| 184 | -0.107471 | -0.517187 | -0.473539 | -0.133990 | -0.148965 | 2.621749  | 0.281129  | -0.237538 | -0.57 |
| 185 | -0.114631 | -0.350905 | -0.402720 | -0.254863 | -0.187989 | 1.563886  | 1.812410  | -0.388373 | -0.58 |
| 186 | -0.165823 | -0.263033 | -0.073894 | -0.333808 | -0.170585 | -0.402311 | 0.006430  | -0.347448 | -0.43 |
| 187 | -0.166312 | -0.217535 | -0.127278 | -0.354470 | -0.188380 | -0.419604 | 0.021133  | -0.344235 | -0.42 |
| 188 | -0.174482 | -0.011065 | -0.153146 | -0.158601 | -0.322998 | 0.202676  | 0.079936  | -0.312336 | -0.42 |
| 189 | -0.176995 | -0.021145 | -0.136286 | -0.047678 | -0.256053 | 0.260258  | 0.115175  | -0.107318 | -0.42 |
| 190 | -0.164317 | -0.182053 | -0.337838 | -0.265893 | -0.267236 | -0.440287 | 0.671119  | -0.286805 | -0.42 |
| 191 | -0.167830 | -0.325988 | -0.284017 | -0.260497 | -0.382963 | -0.311795 | 0.670770  | -0.182638 | -0.46 |
| 192 | -0.096402 | -0.422320 | -0.494245 | 2.889138  | -0.477018 | 0.377125  | 0.522240  | -0.429912 | -0.57 |
| 193 | -0.100391 | -0.378157 | -0.352568 | 2.035244  | -0.439438 | 0.411293  | 0.383717  | -0.274559 | -0.50 |
| 194 | -0.113487 | 0.444467  | -0.549839 | -0.468444 | 0.120016  | 0.582435  | 0.755217  | 0.606611  | -0.65 |
| 195 | -0.117696 | 0.721574  | -0.511333 | -0.326439 | -0.250943 | 0.352607  | 0.454183  | 0.761518  | -0.52 |
| 196 | -0.114942 | -0.160365 | -0.533933 | 0.477747  | -0.362841 | -0.178120 | 1.122167  | -0.011467 | -0.49 |
| 197 | -0.114295 | -0.113225 | -0.417798 | 0.289113  | -0.359780 | -0.035457 | 1.201101  | -0.023936 | -0.52 |

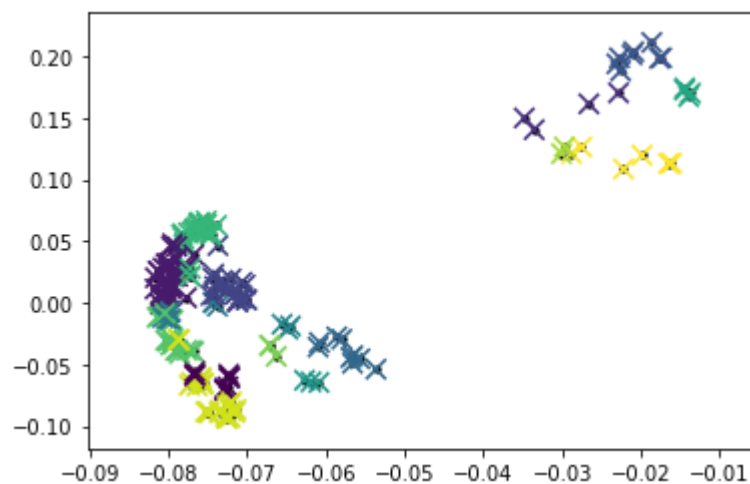
198 rows × 384 columns

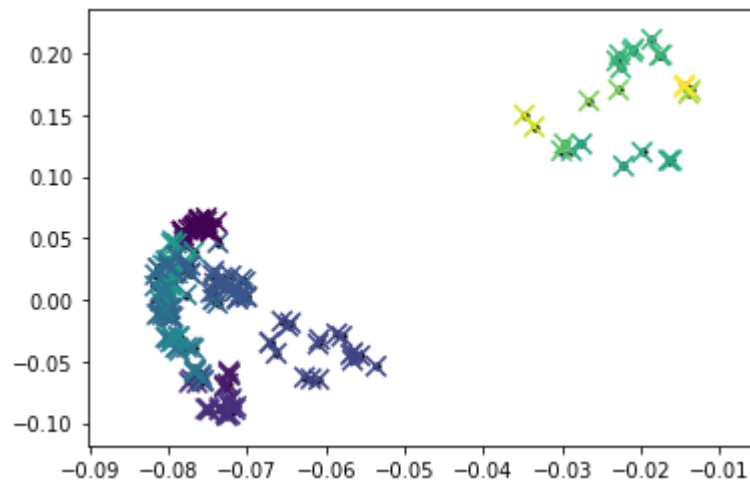


```

1      42
14     27
10     27
3      23
11     19
6       9
5       9
0       9
4       8
15      6
9       4
2       4
12      3
8       3
7       3
13      2
dtype: int64
cancer_non-small cell lung    26
cancer_melanoma              26
cancer_renal                 23
cancer_colon                 21
cancer_ovarian               21
cancer_leukemia              18
cancer_CNS                   18
cancer_breast                15
normal_brain                  8
cancer_prostate               6
normal_blood                  6
normal_ovary                  2
normal_kidney                 2
normal_lung                   2
normal_prostate               2
normal_skin                   2
Name: batch, dtype: int64

```





## Hierarchical Clustering

```

In [5]: from sklearn.cluster import AgglomerativeClustering
single = AgglomerativeClustering(n_clusters=16, linkage='single').fit(expr)
complete = AgglomerativeClustering(n_clusters=16, linkage='complete').fit(expr)
average = AgglomerativeClustering(n_clusters=16, linkage='average').fit(expr)

plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=nci60.batch.astype('category').cat.codes)
plt.title("nci60 ORIGINAL")
plt.show()

plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=complete.labels_)
plt.title("nci60 COMPLETE LINKAGE")
plt.show()

plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=single.labels_)
plt.title("nci60 SINGLE LINKAGE")
plt.show()

plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=average.labels_)
plt.title("nci60 AVERAGE LINKAGE")
plt.show()

# ON YOUR OWN - Explore for synthetic data set (comment nci60 plots and uncomment the ones below)
display(X)
single = AgglomerativeClustering(n_clusters=16, linkage='single').fit(X)
complete = AgglomerativeClustering(n_clusters=16, linkage='complete').fit(X)
average = AgglomerativeClustering(n_clusters=16, linkage='average').fit(X)

#### SYNTHETIC DATA ####
plt.scatter(X[:, 0], X[:, 1], s = 50, c = colors)
plt.title("SYNTHETIC DATA ORIGINAL")
plt.show()

plt.scatter(X[:, 0], X[:, 1], s = 50, c = complete.labels_)
plt.title("SYNTHETIC DATA COMPLETE LINKAGE")
plt.show()

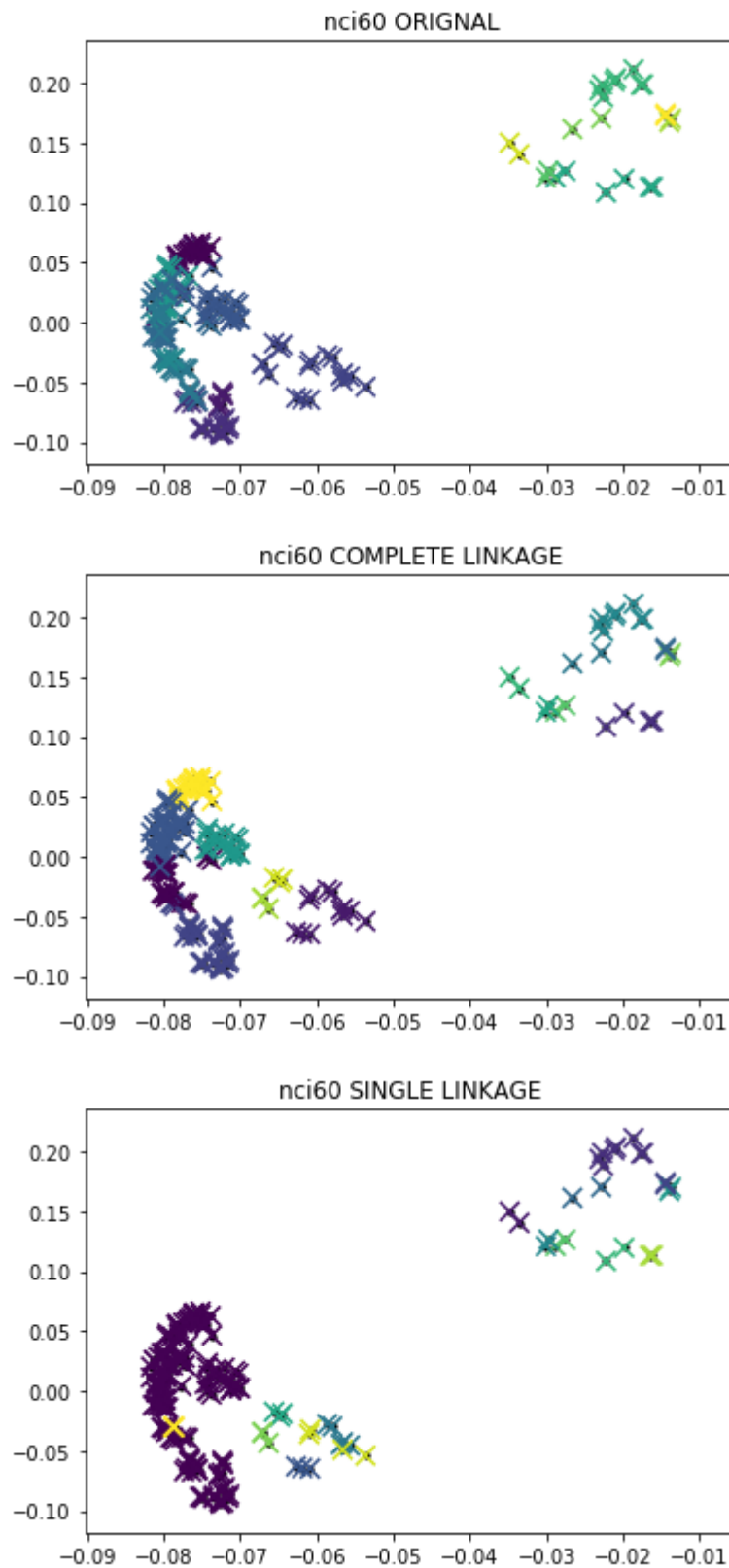
plt.scatter(X[:, 0], X[:, 1], s = 50, c = single.labels_)
plt.title("SYNTHETIC DATA SINGLE LINKAGE")
plt.show()

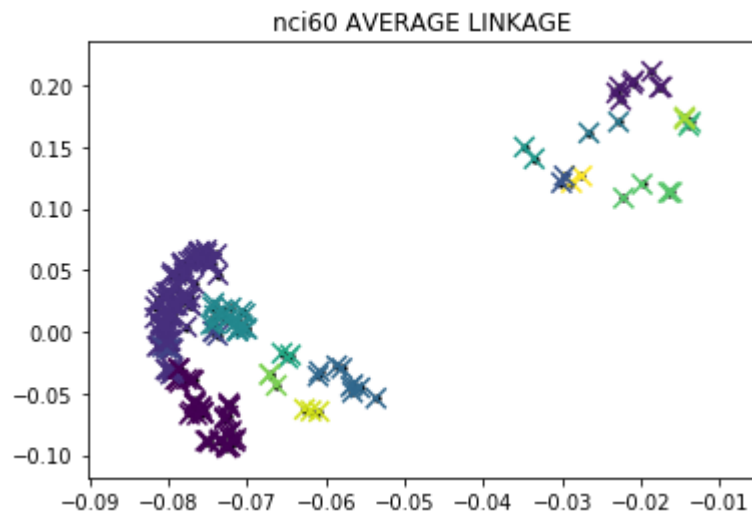
plt.scatter(X[:, 0], X[:, 1], s = 50, c = average.labels_)
plt.title("SYNTHETIC DATA AVERAGE LINKAGE")
plt.show()

# reset assignments back to nci60
from sklearn.cluster import AgglomerativeClustering
single = AgglomerativeClustering(n_clusters=16, linkage='single').fit(expr)

```

```
complete = AgglomerativeClustering(n_clusters=16, linkage='complete').fit(expr)
average = AgglomerativeClustering(n_clusters=16, linkage='average').fit(expr)
```



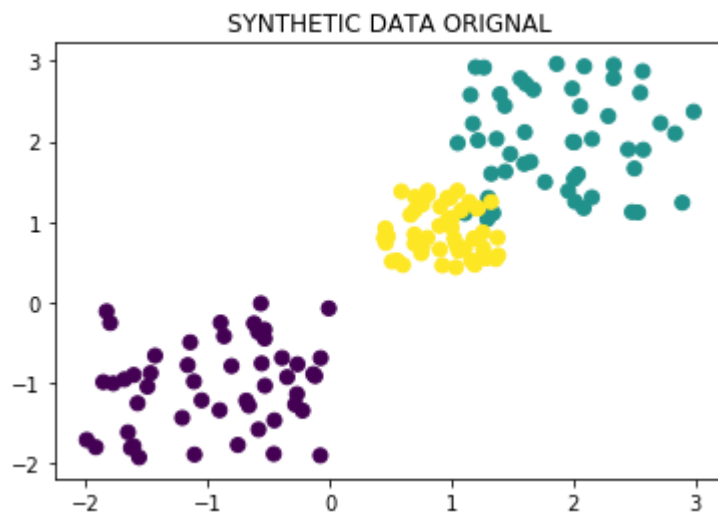


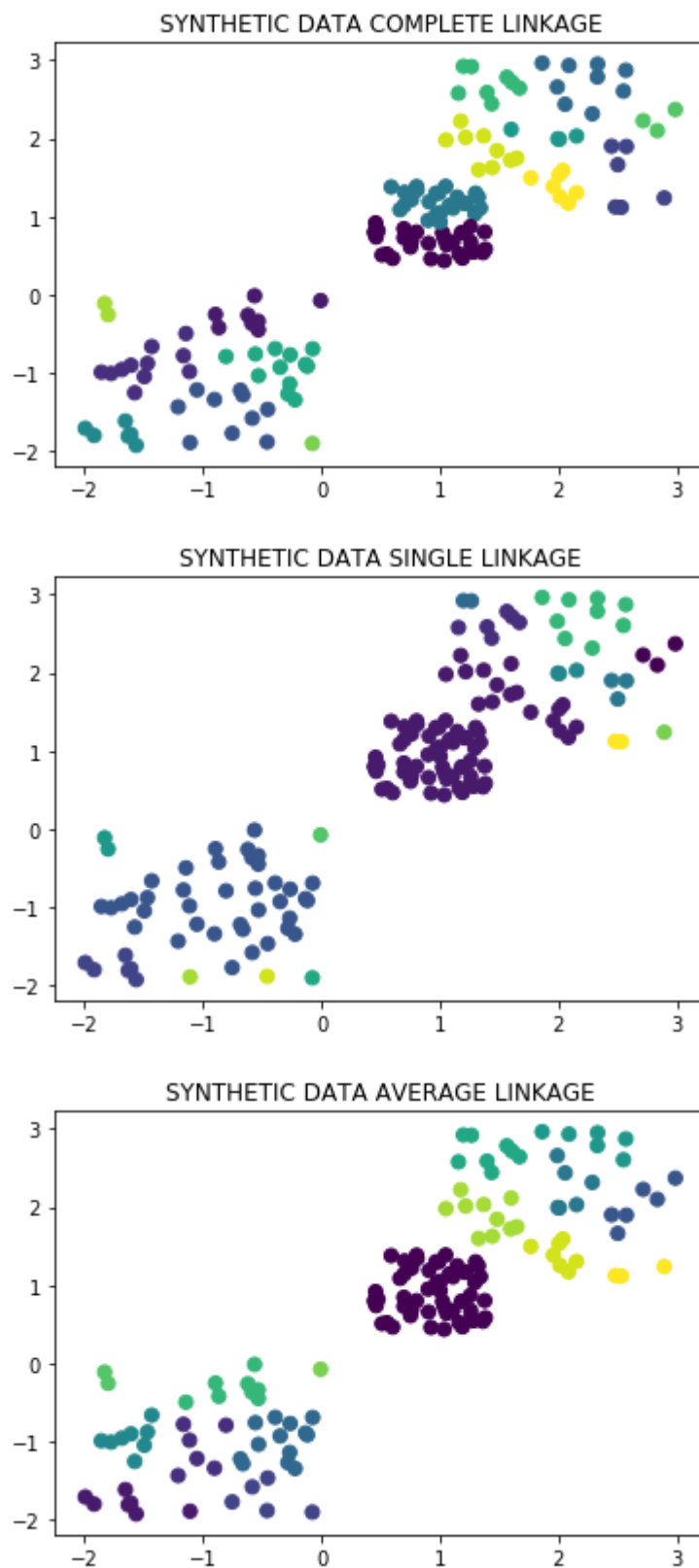
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```



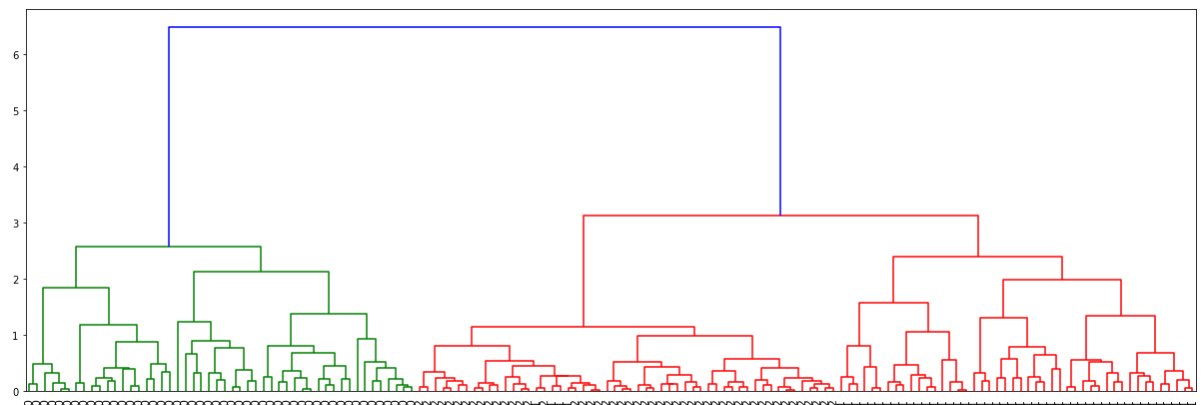


## Hierarchical Clustering with Scipy

```
In [6]: from scipy.cluster.hierarchy import dendrogram, linkage
# cannot choose number of clusters
Z = linkage(expr, 'complete')
# display(Z)
# plt.figure(figsize=(21, 7))
# dendrogram(Z, orientation='top',
#             labels=nci60.tissue,
#             distance_sort='descending',
#             leaf_font_size='11',
#             show_leaf_counts=True)
# plt.show()

# synthetic data
Z = linkage(X, 'complete')
plt.figure(figsize=(21, 7))
dendrogram(Z, orientation='top',
            labels=colors,
            distance_sort='descending',
            leaf_font_size='11',
            show_leaf_counts=True)
plt.show()

# reset back to nci60
Z = linkage(expr, 'complete')
```

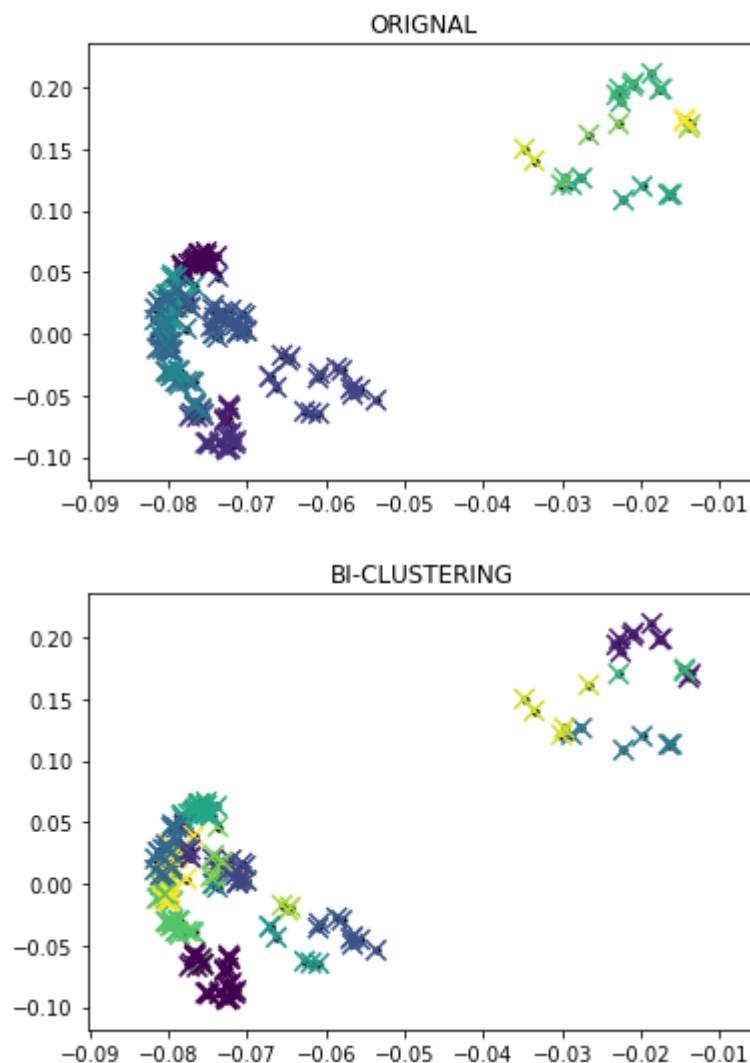


## Bi-Clustering for Omics data

```
In [7]: from sklearn.cluster import SpectralBiclustering
bicluster = SpectralBiclustering(n_clusters=16, random_state=0).fit(expr)

plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=nci60.batch.astype('c
ategory').cat.codes)
plt.title("ORIGINAL")
plt.show()


plt.scatter(nci60.PC2, nci60.PC3, s = 10, c='black')
plt.scatter(nci60.PC2, nci60.PC3, s = 100, marker='x', c=bicluster.row_labels_
)
plt.title("BI-CLUSTERING")
plt.show()
```



# Lab

Try unsupervised learning on the synthetic dataset in Orange

Use code below for the python data widget

 alt text

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from Orange.data import Domain, Table
##### clustering (unsupervised/descrete) #####
# random generated data
# Generating 3 distinct cluster, 2 of them slightly overlapping
X = -2 * np.random.rand(50,2)
X1 = 1 + 2 * np.random.rand(50,2)
X2 = 0.4 + np.random.rand(50,2)

X = np.append(X,X1,axis=0)
X = np.append(X,X2,axis=0)
colors = [0]*50+[1]*50+[2]*50
dfX = pd.DataFrame(X)
dfX['color'] = colors

out_data = Table(dfX)
```