In [1]:
```python
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

from sklearn.neighbors import KNeighborsClassifier
from sklearn.cluster import KMeans
```

1. KNN for Classification

Check the documentation for `sklearn.neighbors.KNeighborsClassifier`. Below are three important parameters:

- **n_neighbors**: int, `default=5`. Number of neighbors to use.
- **p**: int, `default=2`, which means euclidean_distance (l2) will be used. When `p` = 1, use manhattan_distance (l1).
- **weights**: Weight function used in prediction. `Default= ‘uniform’`, which means all neighbors are weighted equally. Other options include `‘distance’`: i.e., weight instances by the inverse of their distance to the new instance (i.e., weighted voting).

Let's use the default setting for modeling and prediction: i.e., euclidean distance with uniform weights for all neighbors.

1.1 Data Preparation

The **iris** data set consists of **4 features for 150 flowers**: Sepal Length, Sepal Width, Petal Length, and Petal Width. The target variable is the **species** of those flowers: `Setosa(0)`, `Versicolour(1)`, and `Virginica(2)`.

Check this link for more details of this dataset.

In [2]:
```python
from sklearn.datasets import load_iris

X, y = load_iris(return_X_y = True, as_frame = True)

display(y.unique(), X.describe())  # display unique values of y,   descriptive stat
```

```
array([0, 1, 2])
```

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)
count	150.000000	150.000000	150.000000	150.000000
mean	5.843333	3.057333	3.758000	1.199333
std	0.828066	0.435866	1.765298	0.762238
min	4.300000	2.000000	1.000000	0.100000
25%	5.100000	2.800000	1.600000	0.300000
50%	5.800000	3.000000	4.350000	1.300000
75%	6.400000	3.300000	5.100000	1.800000
max	7.900000	4.400000	6.900000	2.500000

1.1(a) Split data

In [3]:
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_sta

display(X_train.shape, X_test.shape, y_train.shape, y_test.shape)
```

```
(105, 4)
(45, 4)
(105,)
(45,)
```

1.1(b) Scale features

`StandardScaler` standardizes the data by removing the mean from each value and devide the result by standard deviation. Check documentation for details.

$$z = \frac{x - u}{\sigma}$$

After standardization, the mean of scaled training feature will be 0, and standard deviation will be 1.

- Check the mean (u) and standard deviation (σ) of the scaled test features, why their mean is not 0 and std is not 1?

In [4]:
```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()                              # define the scaler

scaler.fit(X_train)                                    # train the scaler on training
X_train_scaled = scaler.transform(X_train)             # apply the scaler to transform
#X_train_scaled = scaler.fit_transform(X_train)        # combine the above two lines t

X_test_scaled = scaler.transform(X_test)               # apply the scaler to transform
```

```
print("Mean for X_train_scaled: ", X_train_scaled.mean(axis = 0))   # aggregate acr
print("Std for X_train_scaled: ", X_train_scaled.std(axis = 0))
print("Mean for X_test_scaled: ", X_test_scaled.mean(axis = 0))
print("Std for X_test_scaled: ", X_test_scaled.std(axis = 0))
```

```
Mean for X_train_scaled:  [-1.24979392e-15 -4.86383420e-17 -1.14194368e-16  3.024036
05e-16]
Std for X_train_scaled:  [1. 1. 1. 1.]
Mean for X_test_scaled:  [-0.19098204  0.09539869 -0.13098187 -0.12144323]
Std for X_test_scaled:  [0.78888297 0.95940172 0.92394678 0.92084194]
```

1.2 Modeling

1.2(a) Train `m1` with `k` =1

In [5]:
```
m1 = KNeighborsClassifier(n_neighbors=1)

m1.fit(X_train_scaled, y_train)

train_score = m1.score(X_train_scaled, y_train)
test_score = m1.score(X_test_scaled,y_test)

print("1-NN Train Acc: {:.2%}; Test Acc: {:.2%}".format(train_score,test_score))  #
```

```
1-NN Train Acc: 100.00%; Test Acc: 93.33%
```

Check the neighbors

The `kneighbors` method shows the neighbors for given instances: (1) the distance(s) between each instance and its nearest neighbor(s); (2) the index of the neighbor(s) for each instance.

Let's check the training instances' neighbors (can also be applied to test).

- Note that when `k` = 1, the nearest neighbor for a training instance is itself.

In [6]:
```
#m1.kneighbors(X_train_scaled)   # uncomment to see the result: distances are all 0
```

Predict class labels

- Let's apply the model to predict test instance's target value.

In [7]:
```
m1.predict(X_test_scaled)       #  use X_test_scaled for prediction.
```

Out[7]:
```
array([2, 1, 0, 2, 0, 2, 0, 1, 1, 1, 1, 1, 1, 2, 1, 0, 1, 1, 0, 0, 2, 1,
       0, 0, 2, 0, 0, 1, 1, 0, 2, 1, 0, 2, 2, 1, 0, 2, 1, 1, 2, 0, 2, 0,
       0])
```

Estimate class probability

Estimate the class probability for each test instance. **Why the probabilities are either 100% or 0%?**

```
In [8]: m1.predict_proba(X_test_scaled)
```

```
Out[8]: array([[0., 0., 1.],
               [0., 1., 0.],
               [1., 0., 0.],
               [0., 0., 1.],
               [1., 0., 0.],
               [0., 0., 1.],
               [1., 0., 0.],
               [0., 1., 0.],
               [0., 1., 0.],
               [0., 1., 0.],
               [0., 1., 0.],
               [0., 1., 0.],
               [0., 1., 0.],
               [0., 0., 1.],
               [0., 1., 0.],
               [1., 0., 0.],
               [0., 1., 0.],
               [0., 1., 0.],
               [1., 0., 0.],
               [1., 0., 0.],
               [0., 0., 1.],
               [0., 1., 0.],
               [1., 0., 0.],
               [1., 0., 0.],
               [0., 0., 1.],
               [1., 0., 0.],
               [1., 0., 0.],
               [0., 1., 0.],
               [0., 1., 0.],
               [1., 0., 0.],
               [0., 0., 1.],
               [0., 1., 0.],
               [1., 0., 0.],
               [0., 0., 1.],
               [0., 0., 1.],
               [0., 1., 0.],
               [1., 0., 0.],
               [0., 0., 1.],
               [0., 1., 0.],
               [0., 1., 0.],
               [0., 0., 1.],
               [1., 0., 0.],
               [0., 0., 1.],
               [1., 0., 0.],
               [1., 0., 0.]])
```

1.2(b) Train `m2` (k = 5) and `m3` (k = 50)

- Please check the train and test accuracy for each model. Which one is better?

- Estimate the class probabilities for test instances.

Exercise 1: Your Codes Here

```
In [9]:
m2 = KNeighborsClassifier(n_neighbors=5)
m2.fit(X_train_scaled, y_train)
train_score = m2.score(X_train_scaled, y_train)
test_score = m2.score(X_test_scaled,y_test)
print("5-NN Train Acc: {:.2%}; Test Acc: {:.2%}".format(train_score,test_score))
```

```
5-NN Train Acc: 97.14%; Test Acc: 97.78%
```

```
In [10]:
m3 = KNeighborsClassifier(n_neighbors=50)
m3.fit(X_train_scaled, y_train)
train_score = m3.score(X_train_scaled, y_train)
test_score = m3.score(X_test_scaled, y_test)
print("50-NN Train Acc: {:.2%}; Test Acc: {:.2%}".format(train_score,test_score))
```

```
50-NN Train Acc: 84.76%; Test Acc: 86.67%
```

```
In [ ]:
```

```
In [ ]:
```

1.3 GridSearchCV

- Bigger `k` values: more neighbors used in prediction, simpler model (decision boundary).
- Smaller `k` values: less neigbors used, more complicated model which tends to overfit.

```
In [11]:
from sklearn.model_selection import GridSearchCV

knn = KNeighborsClassifier()

k_range = {'n_neighbors': np.arange(1,84,2)}                          #  k = 1,3,

grid = GridSearchCV(estimator = knn, param_grid = k_range, cv = 5)      # 5-CV on t

grid.fit(X_train_scaled, y_train)       # search over the values on Train data (wit

best_param = grid.best_params_          # k value that returns highest mean cv scor
best_cv_score = grid.best_score_        # mean cv score of the best k

print("Best Params: {}".format(best_param))
print("Mean cv score of the best k: {:.2%}".format(best_cv_score))
```

```
c:\Users\betoq\anaconda3\Lib\site-packages\joblib\externals\loky\backend\context.py:
136: UserWarning: Could not find the number of physical cores for the following reas
on:
[WinError 2] El sistema no puede encontrar el archivo especificado
Returning the number of logical cores instead. You can silence this warning by setti
ng LOKY_MAX_CPU_COUNT to the number of cores you want to use.
  warnings.warn(
  File "c:\Users\betoq\anaconda3\Lib\site-packages\joblib\externals\loky\backend\con
text.py", line 257, in _count_physical_cores
    cpu_info = subprocess.run(
        "wmic CPU Get NumberOfCores /Format:csv".split(),
        capture_output=True,
        text=True,
    )
  File "c:\Users\betoq\anaconda3\Lib\subprocess.py", line 554, in run
    with Popen(*popenargs, **kwargs) as process:
         ~~~~~^^^^^^^^^^^^^^^^^^^^^^
  File "c:\Users\betoq\anaconda3\Lib\subprocess.py", line 1039, in __init__
    self._execute_child(args, executable, preexec_fn, close_fds,
    ~~~~~~~~~~~~~~~~~~~^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
                        pass_fds, cwd, env,
                        ^^^^^^^^^^^^^^^^^^^
    ...<5 lines>...
                        gid, gids, uid, umask,
                        ^^^^^^^^^^^^^^^^^^^^^^
                        start_new_session, process_group)
                        ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File "c:\Users\betoq\anaconda3\Lib\subprocess.py", line 1554, in _execute_child
    hp, ht, pid, tid = _winapi.CreateProcess(executable, args,
                       ~~~~~~~~~~~~~~~~~~~~~^^^^^^^^^^^^^^^^^^
                             # no special security
                             ^^^^^^^^^^^^^^^^^^^^^
    ...<4 lines>...
                             cwd,
                             ^^^^
                             startupinfo)
                             ^^^^^^^^^^^^
Best Params: {'n_neighbors': np.int64(5)}
Mean cv score of the best k: 95.24%
```

1.3(a) Visualize mean cv scores for each k value

Use `matplotlib.pyplot.plot` function (check documentation) to create a line (i.e., the model). By default, a solid blue line is created to connect all points.

- `x` : the horizontal coordinate of the data points.
- `y` : the vertical coordinate of the data points.

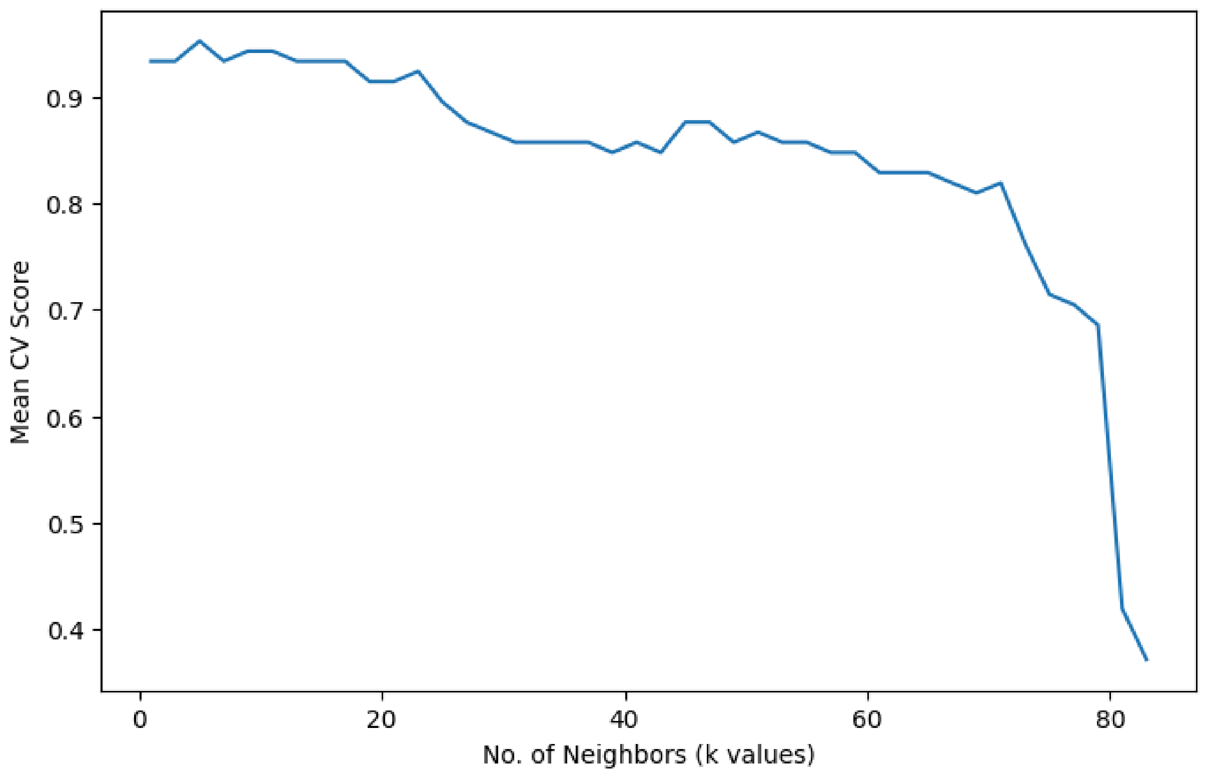
Note the function relies on **positional arguments** for `x`, `y` (and `fmt`), NOT **keyword argument**, therefore there is no need to specify the parameter names.

- Other keyword parameters such as `linewidth`, `markersize`, `color` / `c` (which override the color in `fmt`) should be placed after positional paramters.

In [12]:
```
k_values = grid.cv_results_['param_n_neighbors']        # k values, same as k_range
cv_scores = grid.cv_results_['mean_test_score']         # mean cv scores for each k

plt.figure(figsize = (8, 5))
plt.plot(k_values,  cv_scores)        # a line plot (default blue solid line)
plt.xlabel('No. of Neighbors (k values)')
plt.ylabel('Mean CV Score')
plt.title('k-NN: Best k = {} & Mean CV Score : {:.2%}'.format(best_param['n_neighbo
plt.show()
```

k-NN: Best k = 5 & Mean CV Score : 95.24%



1.3(b) Evaluate and apply the best model

- Note that the best model was refitted on entire training data in the search process.

```
In [13]: grid.score(X_test_scaled,y_test)     #check the best model's generalization perform

         #Alternatively
         #knn_best = grid.best_estimator_
         #knn_best.score(X_test_scaled,y_test)
```

```
Out[13]: 0.9777777777777777
```

```
In [14]: grid.predict(X_test_scaled)          # class predictions on test set
```

```
Out[14]: array([2, 1, 0, 2, 0, 2, 0, 1, 1, 1, 2, 1, 1, 1, 1, 0, 1, 1, 0, 0, 2, 1,
                0, 0, 2, 0, 0, 1, 1, 0, 2, 1, 0, 2, 2, 1, 0, 2, 1, 1, 2, 0, 2, 0,
                0])
```

```
In [15]: grid.predict_proba(X_test_scaled)   # class probability estimation test set
```

```
Out[15]: array([[0. , 0. , 1. ],
               [0. , 1. , 0. ],
               [1. , 0. , 0. ],
               [0. , 0. , 1. ],
               [1. , 0. , 0. ],
               [0. , 0. , 1. ],
               [1. , 0. , 0. ],
               [0. , 1. , 0. ],
               [0. , 0.8, 0.2],
               [0. , 1. , 0. ],
               [0. , 0.2, 0.8],
               [0. , 1. , 0. ],
               [0. , 0.8, 0.2],
               [0. , 0.6, 0.4],
               [0. , 0.8, 0.2],
               [1. , 0. , 0. ],
               [0. , 0.6, 0.4],
               [0. , 1. , 0. ],
               [1. , 0. , 0. ],
               [1. , 0. , 0. ],
               [0. , 0. , 1. ],
               [0. , 1. , 0. ],
               [1. , 0. , 0. ],
               [1. , 0. , 0. ],
               [0. , 0. , 1. ],
               [1. , 0. , 0. ],
               [1. , 0. , 0. ],
               [0. , 0.8, 0.2],
               [0. , 1. , 0. ],
               [1. , 0. , 0. ],
               [0. , 0.2, 0.8],
               [0. , 1. , 0. ],
               [1. , 0. , 0. ],
               [0. , 0.4, 0.6],
               [0. , 0. , 1. ],
               [0. , 1. , 0. ],
               [1. , 0. , 0. ],
               [0. , 0.2, 0.8],
               [0. , 0.8, 0.2],
               [0. , 1. , 0. ],
               [0. , 0. , 1. ],
               [1. , 0. , 0. ],
               [0. , 0. , 1. ],
               [1. , 0. , 0. ],
               [1. , 0. , 0. ]])
```

2. K-Means Clustering

2.1 Data Preparation

The **Wholesale Customer Data** comes from the Machine Learning Data Repository of UC Irvine. Check this link for more details

- Here we removed 19 outliers for simplicity, so the data contains only 421 instances.

There are in total 8 variables:

- `Channel` : Horeca (Hotel/Restaurant/Cafe) or Retail channel (Categorical);
- `Region` : Lisnon, Oporto or Other (Categorical);
- `Fresh` : annual spending on fresh products (Continuous);
- `Milk` : annual spending on milk products (Continuous);
- `Grocery` : annual spending on grocery products (Continuous);
- `Frozen` : annual spending on frozen products (Continuous);
- `Detergents_Paper` : annual spending on detergents and paper products (Continuous);
- `Delicassen` : annual spending on and delicatessen products (Continuous);

We'd like to group those customers into different clusters according to their purchasing patterns. **As here we only want to explore the underlying structure of our customers, here we use the entire dataset in model training.**

In [16]:
```
cust_df = pd.read_csv('Wholesale_customers_v2.csv')   # modify data path if needed

X = cust_df.drop(columns = ['Channel', 'Region'])     # remove two irrelant columns

display(X.shape, X.head())
```

```
(421, 6)
```

	Fresh	Milk	Grocery	Frozen	Detergents_Paper	Delicassen
0	12669	9656	7561	214	2674	1338
1	7057	9810	9568	1762	3293	1776
2	6353	8808	7684	2405	3516	7844
3	13265	1196	4221	6404	507	1788
4	22615	5410	7198	3915	1777	5185

Scale the Data

In [17]:
```
scaler = StandardScaler()

X_scaled = scaler.fit_transform(X)                            # fit/transform on t

X_scaled = pd.DataFrame(data = X_scaled, columns = X.columns)  # convert the array

X_scaled.describe()   # After standardization: mean = 0, std = 1
```

Out[17]:

	Fresh	Milk	Grocery	Frozen	Detergents_Paper	D
count	4.210000e+02	4.210000e+02	4.210000e+02	4.210000e+02	4.210000e+02	4.21
mean	1.265812e-17	5.063250e-17	-8.438750e-18	5.063250e-17	6.751000e-17	4.64
std	1.001190e+00	1.001190e+00	1.001190e+00	1.001190e+00	1.001190e+00	1.00
min	-1.078911e+00	-1.002890e+00	-1.012455e+00	-8.594059e-01	-7.087221e-01	-1.01
25%	-7.713914e-01	-7.179169e-01	-7.082173e-01	-6.380164e-01	-6.382488e-01	-6.97
50%	-2.722736e-01	-3.024545e-01	-3.595431e-01	-3.812313e-01	-4.836532e-01	-2.92
75%	4.879954e-01	3.797366e-01	4.018331e-01	2.148174e-01	3.609123e-01	3.51
max	4.260736e+00	4.914126e+00	4.622410e+00	5.098075e+00	4.697110e+00	5.31

2.2 Modeling

The `sklearn.cluster.KMeans` function find cluster centroids that minimise the **inertia** or **SSE**.

- **n_clusters**: int, `default=8`. The number of clusters to form.
- **init**: method for initialization, `default='k-means++'` pushes the centroids as far as possible from each other. Other options include `'random'` or any array.
- **n_init**: int, the number of iterations the algorithm will be run with different initial centroids, that returns the best output after `n_init` consecutive runs will be the used as initial centroids. By `default = 'auto'`: i.e., 10 if `init='random'`; 1 if `init='k-means++'` or an array-like.
- **random_state**: int, `default = None`, it determines the random number generation for centroid initialization.
- **max_iter**: int, `default=300`, the maximum number of iterations of the algorithm for a single run.
- **tol**: float, `default=1e-4`, the minimum SSE change between two consecutive iterations to declare convergence.

Check the documentation for details.

2.2(a) Train a model `model` with `k` = 2

- Let's use two features `Fresh` & `Milk` only.

In [18]:
```
X_sub = X_scaled[['Fresh','Milk']]                          # 2D array
```

```
kmeans = KMeans(n_clusters = 2, random_state = 0)      # set random_state for repro

kmeans.fit(X_sub)

kmeans.n_iter_             #  iterations taken to converge
```

```
c:\Users\betoq\anaconda3\Lib\site-packages\sklearn\cluster\_kmeans.py:1419: UserWarn
ing: KMeans is known to have a memory leak on Windows with MKL, when there are less
chunks than available threads. You can avoid it by setting the environment variable
OMP_NUM_THREADS=2.
  warnings.warn(
```

```
Out[18]:  6
```

2.2(b) Cluster allocation and clustering quality

Cluster Allocation

Cluster labels will be assigned to each instance automatically in model training process, the labels can be obtained with `.labels_` attribute.

- When apply the model to predict the cluster labels for new instances, use the `predict` method.

```
In [19]: kmeans.labels_                # cluster labels (for training instances)

         #kmeans.predict(X_sub)        # same as above
```

```
Out[19]: array([0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 1, 0, 1, 0,
                1, 1, 1, 0, 1, 0, 1, 1, 0, 1, 1, 0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 0,
                0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1,
                0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0,
                0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 1, 1, 1, 0, 0, 0, 1, 0, 1,
                0, 0, 0, 1, 1, 1, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 0,
                1, 1, 0, 0, 0, 1, 1, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0,
                0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
                1, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0,
                0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 1,
                0, 0, 1, 0, 1, 1, 1, 1, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 1, 0, 1, 0,
                0, 1, 0, 0, 1, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 1, 0, 0, 1, 0, 0, 1,
                0, 0, 1, 1, 1, 0, 1, 1, 1, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 1, 0, 0,
                0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1,
                0, 0, 1, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0,
                0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1,
                1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 1, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0,
                1, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0,
                0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 0, 0, 1, 0, 0, 0, 0, 1, 0, 1, 1, 1,
                0, 0, 0], dtype=int32)
```

Clustering Quality

Clustering quality is measured by **SSE/Inertia**, which is obtained with the `.inertia_` attribute.

- The `.score` method will return the opposite of SSE (a negative SSE): larger scores means better clustering quality. It is useful in GridSearch and Cross-validation.

In [20]:
```
kmeans.inertia_                # SSE: the smaller, the better the model is

#kmeans.score(X_sub)           # score: negative SSE (the bigger, the better the mode
```

Out[20]:
```
546.7008974797891
```

2.2(c) Check cluster centroids

The centroids are usually the **means feature values of instances in the same cluster**, which can be obtained with the `.cluster_centers_` attribute.

- Note if the algorithm stops before fully converging (due to the setting of `tol` or `max_iter`), the `cluster_centers_` are NOT the means of instances in each cluster (i.e., cluster means).

  The reason is in the last iteration, the model stops after cluster allocation, then the cluster centroids will not be updated with the new means.

- Here our algorithm has been fully converged (i.e., no change in the cluster centroids in the last iteration).

In [21]:
```
centroids = kmeans.cluster_centers_      # cluster centroids, save for later use
centroids

# alternatively, caculate the centroids mannually
#[X_sub.loc[kmeans.labels_ == 0,'Fresh'].mean(), X_sub.loc[kmeans.labels_ == 0,'Mil
#[X_sub.loc[kmeans.labels_ == 1,'Fresh'].mean(), X_sub.loc[kmeans.labels_ == 1,'Mil
```

Out[21]:
```
array([[-0.5211405 ,  0.12087991],
       [ 1.27722138, -0.29625486]])
```

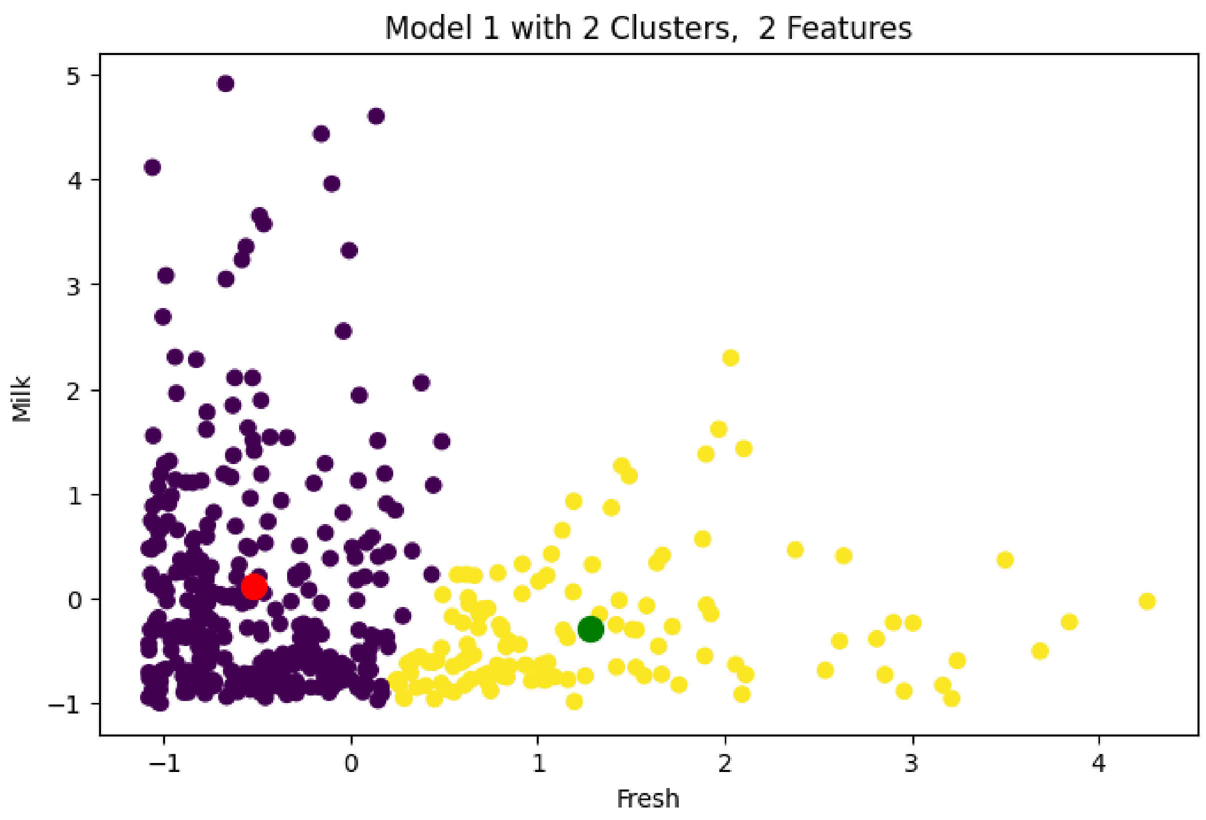
2.2(d) Visualize data and cluster centroids

- Use `matplotlib.pyplot.scatter` function to create scatter plots. Check documentation for details.

In [22]:
```
df = X_sub.copy()                        # create a copy to avoid warning message (op

df['cluster'] = kmeans.labels_           # save cluster labels for each instance in a

plt.figure(figsize = (8, 5))
plt.scatter(x = df['Fresh'], y = df['Milk'], c = df['cluster'])              # map 
plt.scatter(x = centroids[0,0], y = centroids[0,1], c = 'red', s = 100)      # mark
plt.scatter(x = centroids[1,0], y = centroids[1,1], c = 'green', s = 100)    # mark
plt.xlabel("Fresh")
plt.ylabel("Milk")
plt.title('Model 1 with 2 Clusters,  2 Features')
plt.show()
```



2.3 Find the Best `k` Value

Now let's try all 6 features here: i.e., use `X_scaled` in modeling.

2.3(a) The elbow method

The elbow method compares the **clustering quality** for k-means with different k values (often on the training data itself) and choose the **minimum k** value which yields a **relatively low SSE**.

In [23]:
```
k_range = np.arange(1, 31, 1)       # compare 30 k values: 1,2,3..,30

SSEs = []              # create an empty list
for k in k_range:    # loop over all k values
    model = KMeans(n_clusters = k, random_state = 0).fit(X_scaled)      # train the
    SSEs.append(model.inertia_)                                          # append SS

len(SSEs)              # how many SSE are there?
```

```
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```

```
Out[23]: 30
```

Again, we use `matplotlib.pyplot.plot` function (check documentation) to create a line plot. A simple way to adjust the line and marker is format string (`fmt`).

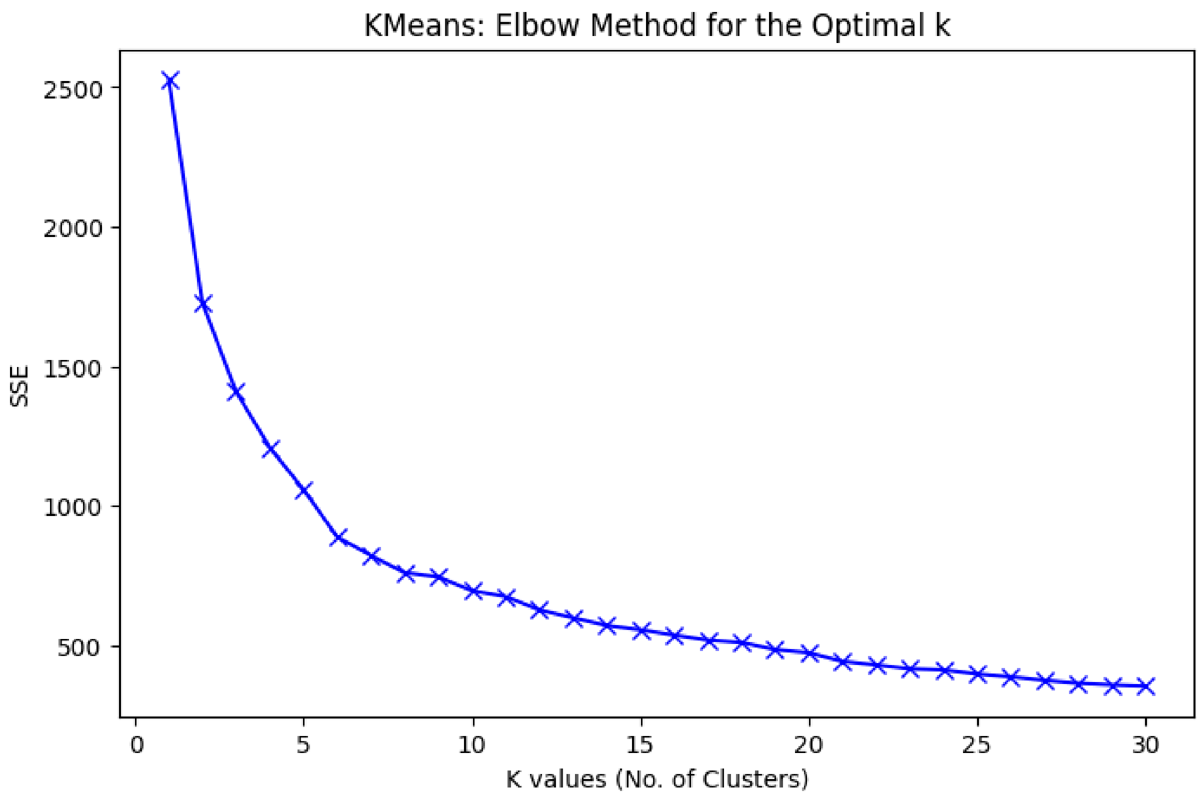
- `fmt` : optional, a format string consists of color, marker and line.

Note the function relies on **positional arguments** for `x` , `y` (and `fmt`), NOT **keyword argument**, therefore there is no need to specify the parameter names.

- Other keyword parameters such as `linewidth` , `markersize` , `color` / `c` (which override the color in `fmt`) should be placed after positional paramters.

```
In [24]: # visualize the plot

plt.figure(figsize = (8,5))
plt.plot(k_range, SSEs,  'bx-',  markersize = 7)                    # 'bx-': blue
#plt.plot(k_range, SSEs, c = 'blue', linestyle = '-', marker = 'x', markersize = 7)
plt.xlabel("K values (No. of Clusters)")
plt.ylabel("SSE")
plt.title('KMeans: Elbow Method for the Optimal k')
plt.show()
```



2.3(b) The GridSearchCV method

Exercise 2: Your Codes Here

Please perform `GridSearchCV` with 5-fold cv on `X_scaled` to find the best `k` from the same range as 2.3(a), use the same random state.

- Check the best k value and its mean cv score during cross-validation. **Does the best k value make sense?**
- Visualize the mean cv scores againt the k values.

Note the `GridSearchCV` function compares **the mean generalization score (i.e., negative SSE)** in cross-validation.

In [25]:
```
model = KMeans(n_clusters = 5, random_state = 0)   # define the model with k = 5
k_range = {"n_clusters": np.arange(1, 31, 1)}                            # k = 1,2,
grid2 = GridSearchCV(estimator = model, param_grid = k_range, cv = 5)      # 5-CV o
grid2.fit(X_scaled)         # search over the values on the entire data (with 5-cv)
best_param2 = grid2.best_params_          # k value that returns highest mean cv sc
best_cv_score2 = grid2.best_score_        # mean cv score of the best k
```

```
print("Best Params: {}".format(best_param2))
print("Mean cv score of the best k: {:.2%}".format(best_cv_score2))
k_values2 = grid2.cv_results_['param_n_clusters']        # k values, same as k_rang
cv_scores2 = grid2.cv_results_['mean_test_score']         # mean cv scores for each
plt.figure(figsize = (8, 5))
plt.plot(k_values2,  cv_scores2)        # a line plot (default blue solid line)
plt.xlabel('No. of Clusters (k values)')
plt.ylabel('Mean CV Score')
plt.title('KMeans Clustering: CV Score vs. k')
plt.grid()
plt.show()
grid2.best_estimator_.inertia_     #check the best model's SSE
```

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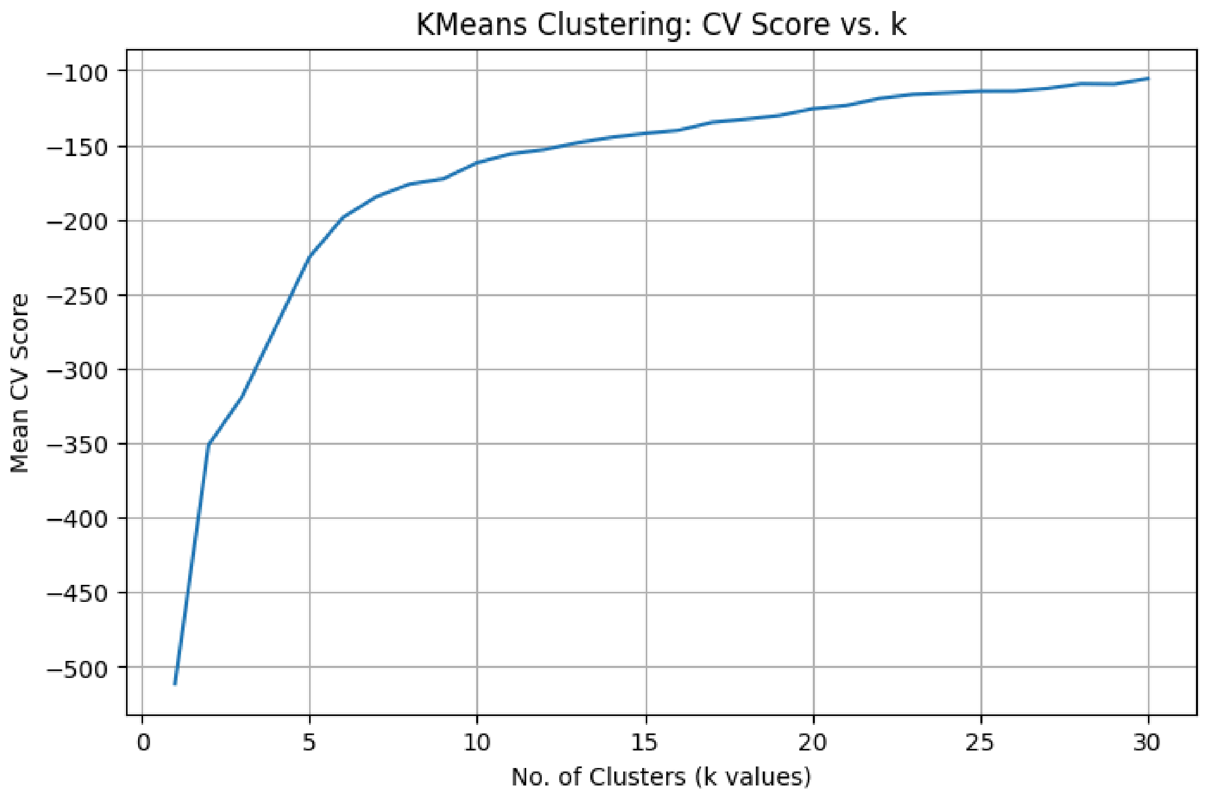
Best Params: {'n_clusters': np.int64(30)}
Mean cv score of the best k: -10549.20%
```



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Out[25]:  355.19401237399
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In [ ]:
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