Artificial Intelligence and Machine Learning

Unit II

Clustering with K-means

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My own latex definitions

In [1]:
```
import matplotlib
import matplotlib.pyplot as plt
import numpy as np
%matplotlib inline
plt.style.use('seaborn-whitegrid')

font = {'family' : 'Times',
        'weight' : 'bold',
        'size'   : 12}

matplotlib.rc('font', **font)


# Aux functions

def plot_grid(Xs, Ys, axs=None):
    ''' Aux function to plot a grid'''
    t = np.arange(Xs.size) # define progression of int for indexing colormap
    if axs:
        axs.plot(0, 0, marker='*', color='r', linestyle='none') #plot origin
        axs.scatter(Xs,Ys, c=t, cmap='jet', marker='.') # scatter x vs y
        axs.axis('scaled') # axis scaled
    else:
        plt.plot(0, 0, marker='*', color='r', linestyle='none') #plot origin
        plt.scatter(Xs,Ys, c=t, cmap='jet', marker='.') # scatter x vs y
        plt.axis('scaled') # axis scaled

def linear_map(A, Xs, Ys):
    '''Map src points with A'''
    # [NxN,NxN] -> NxNx2 # add 3-rd axis, like adding another layer
    src = np.stack((Xs,Ys), axis=Xs.ndim)
    # flatten first two dimension
    # (NN)x2
    src_r = src.reshape(-1,src.shape[-1]) #ask reshape to keep last dimension and adjust the rest
    # 2x2 @ 2x(NN)
    dst = A @ src_r.T # 2xNN
    #(NN)x2 and then reshape as NxNx2
    dst = (dst.T).reshape(src.shape)
    # Access X and Y
    return dst[...,0], dst[...,1]


def plot_points(ax, Xs, Ys, col='red', unit=None, linestyle='solid'):
    '''Plots points'''
    ax.set_aspect('equal')
    ax.grid(True, which='both')
    ax.axhline(y=0, color='gray', linestyle="--")
    ax.axvline(x=0, color='gray',  linestyle="--")
    ax.plot(Xs, Ys, color=col)
    if unit is None:
        plotVectors(ax, [[0,1],[1,0]], ['gray']*2, alpha=1, linestyle=linestyle)
    else:
        plotVectors(ax, unit, [col]*2, alpha=1, linestyle=linestyle)

def plotVectors(ax, vecs, cols, alpha=1, linestyle='solid'):
    '''Plot set of vectors.'''
    for i in range(len(vecs)):
        x = np.concatenate([[0,0], vecs[i]])
        ax.quiver([x[0]],
                  [x[1]],
                  [x[2]],
                  [x[3]],
                  angles='xy', scale_units='xy', scale=1, color=cols[i],
                  alpha=alpha, linestyle=linestyle, linewidth=2)
```

OPIS for Course Evaluation

OPIS CODE: 4UZC1KQA

The code and guide are in the google classroom!

Guide on how to evaluate with OPIS (Opinion of the students):

https://www.uniroma1.it/sites/default/files/field_file_allegati/vademecum_per_studenti_opis_2023_24_1.pdf

https://www.uniroma1.it/sites/default/files/field_file_allegati/guided_path_to_access_student_s_opinions_questionnaire_2023_2024.pdf

Your turn: Self-assessment test + Coding Session Thur, April 11

On next Thursday 11 April 2024 at 2pm we will do a self-assessment test to evaluate yourself on this first part of the program.

Please fill this form https://forms.gle/zsptFtQ6cdQQ1WA89 by **Wed. 10 April @ 3pm**

- 1h 20min Self-Assessment
- 1h 30min Coding

Please bring:

- scientific calculator
- a blue or black pen
- sheet of paper (white or squared) I may bring some too if you do not have.
- your laptop (for the Colab session)

Self-Assessment will cover the first part on:

- vectors, LA, calculus
- PCA, Eigendecomposition, SVD, covariance matrix etc
- Kmeans etc

Recap previous lecture

- Principal Components Analysis (PCA)
- Eigendecomposition of a matrix
- Geometry behind PCA
- Application of PCA for:
  - Compressing the data (point cloud to line)
  - Modeling 3D Faces (3D Morphable Model 3DMM)
  - Rotating the data

Today's lecture

Unsupervised Learning: Clustering

K-means

Coordinate Descent

Application: Pixel Segmentation

Image recognition: Visual Bag of Words (hints)

This lecture material is taken from

- Cimi Book - Chapter 15
- Bishop - Chapter 9.1
- Stanford Kmeans
- Stanford Kmeans
- Illustrations
- Code

Unsupervised Learning

Objective and Motivation: The goal of unsupervised learning is to find **hidden patterns** in unlabeled data.

$$\underbrace{\{\mathbf{x}_i\}_{i=1}^N}_{\text{known}} \sim \underbrace{\mathrm{D}}_{\text{unknown}}$$

- Unlike in supervised learning, any data points is not paired with a label.
- As you can see the unsupervised learning problem is ill-posed (which hidden patterns?) and in principle more difficult than supervised learning.
- Unsupervised learning can be thought of as "finding structure" in the data.

Unsupervised Learning

- PCA and matrix factorization methods such as Eigendecomposition and Singular Value Decomposition (SVD)
- "Hidden Patterns" and "Finding Structure" translate into find a **low dimensional embedding** of the data.
- Usage:
  - Visualization of high dimensional data
  - Dimensionality Reduction
  - Compression and Noise Filtering
  - Further pre-processing by machine learning algorithms
  - Decorrelate the features (i.e. *covariance matrix is diagonal*)

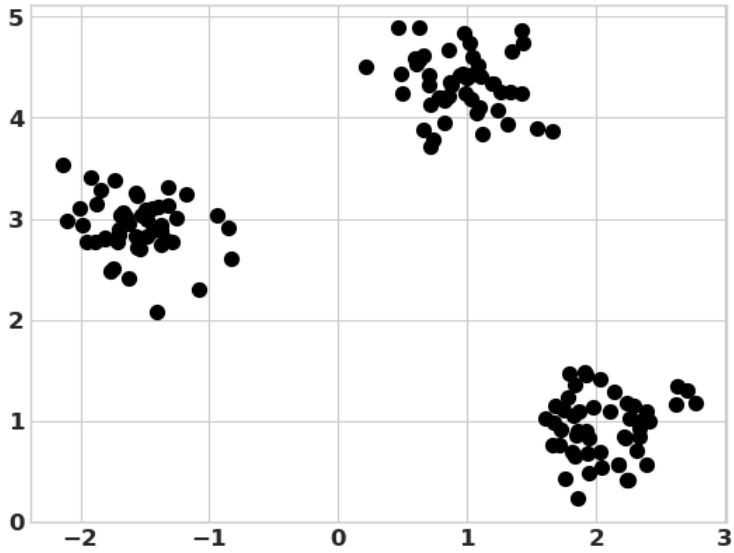
In [2]:
```
from sklearn.datasets import make_blobs

X, y = make_blobs(n_samples=150,
                  n_features=2,
                  centers=3,
                  cluster_std=0.3,
                  shuffle=True,
                  random_state=0)
```

Unsupervised Learning: Clustering

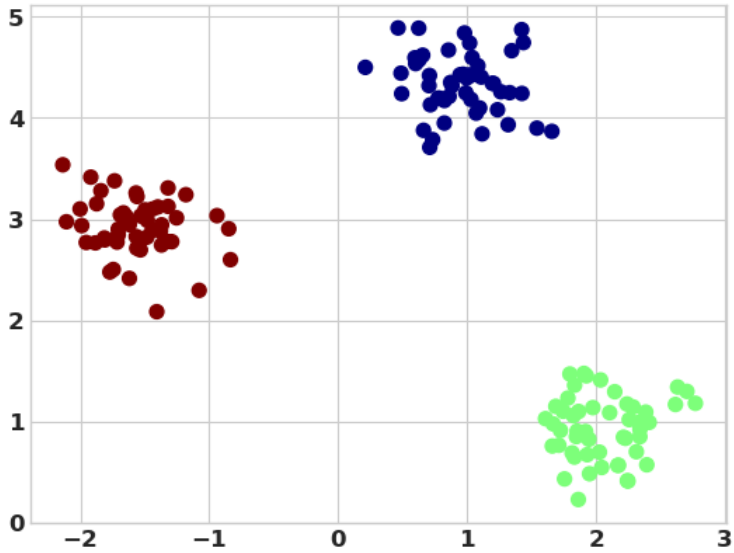
- "Hidden Patterns" and "Finding Structure" translate into **deriving a partitioning of the data into clusters**.

In [3]:
```
plt.scatter(X[:, 0], X[:, 1], c='black', marker='o', s=50)
plt.show()
```

```
findfont: Font family ['Times'] not found. Falling back to DejaVu Sans.
```



In [4]:
```
plt.scatter(X[:, 0], X[:, 1], c=y, marker='o', s=50, cmap='jet')
plt.show()
```



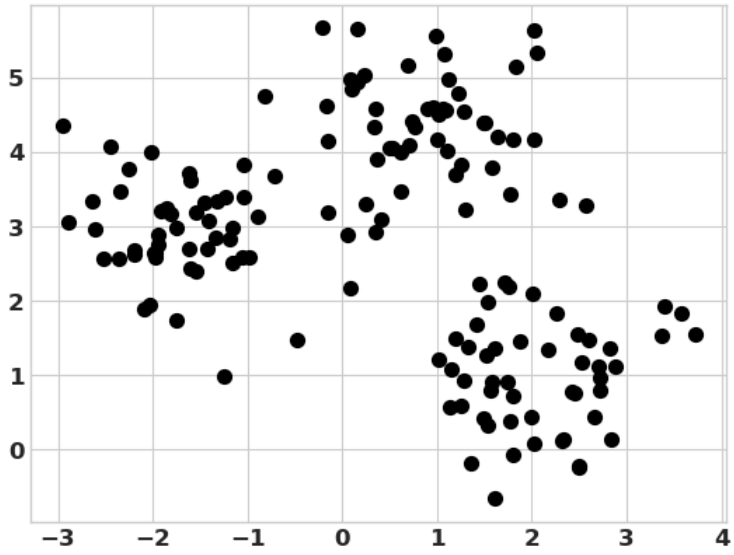
In [5]:
```
from sklearn.datasets import make_blobs

X, y = make_blobs(n_samples=150,
                  n_features=2,
                  centers=3,
                  cluster_std=0.5,
                  shuffle=True,
                  random_state=0)
```

Supervised Learning is more constrained

- The mapping data to color (labels) is given
- With clustering we are given just a point cloud of data with no label assigned

Clustering is ill-posed

In [6]:
```
from sklearn.datasets import make_blobs

X2, y2 = make_blobs(n_samples=150,
                  n_features=2,
                  centers=3,
                  cluster_std=.7,
                  shuffle=True,
                  random_state=0)

plt.scatter(X2[:, 0], X2[:, 1], c='black', marker='o', s=50)
plt.show()
```



- How many cluster here, three or two?

Why Clustering is useful

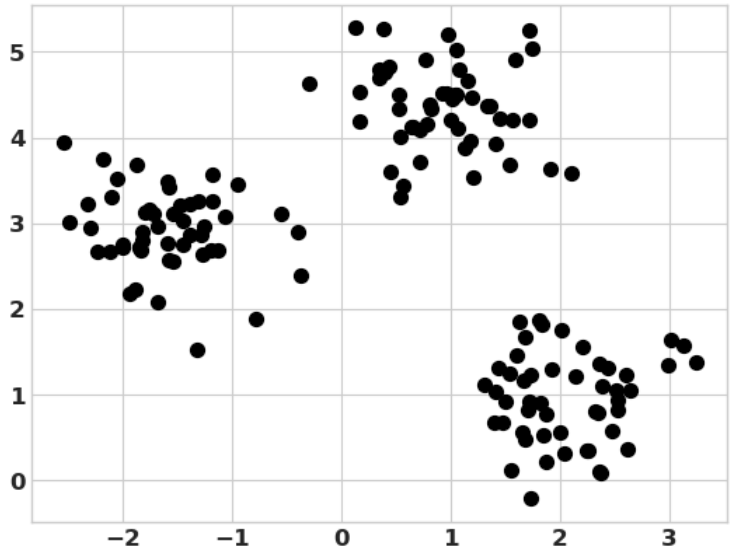
- Applications:
  - Color Compression
  - Vector "quantization"
  - Data compression
  - Image Retrieval (codebook) --> Bag of Visual Words
  - Finding "groups" given points in a vector space
    - I.e. Marketing Department: you have a customer as a vector.
      - Each axis of the vector indicates 1) annual income 2) Age 3) Location etc.
      - Objective: Identify "groups" of customers to have ad-hoc advertising campaign.

Clustering: formalizing the problem

- **Input**:
  1. A set of points $\{\mathbf{x}_1, \ldots, \mathbf{x}_\mathbf{n}\}$ in a d-dim vector space $\mathbf{x} \in \mathrm{R}^d$,
  2. k number of clusters to find

- **Output**:
  1. A set of points **"centroids"** $\{\mu_1, \ldots, \mu_k\}$ where $\mu \in \mathrm{R}^d$,
  2. A list of **assignment labels** that create a **mapping from data points to centroids** $\{y_1, \ldots, y_n\}$
  3. The clusters are meant to be disjoint (there is no overlap between clusters).
     - Note that y is a scalar $\in [1, \ldots, k]$
     - The assignment labels maps a data point to a single centroid
     - It conveys the information: `data points 3 maps to the cluster centroid 2`
     - For this to work formally the y_i needs to be aligned with $\mathbf{x}_i$

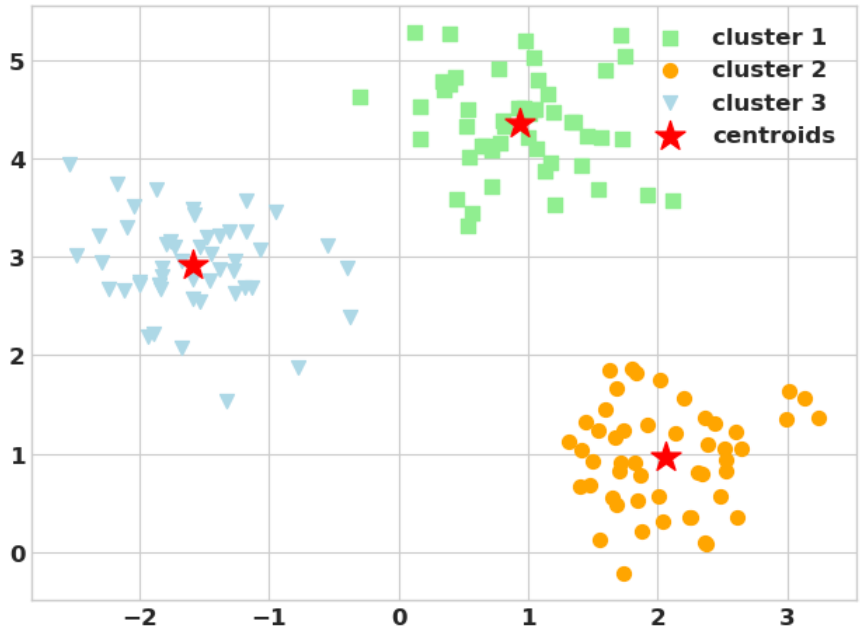
In [7]:
```
plt.scatter(X[:, 0], X[:, 1], c='black', marker='o', s=50)
plt.show()
```



In [8]:

```
from sklearn.cluster import KMeans

km = KMeans(n_clusters=3,
            init='random',
            n_init=10,
            max_iter=300,
            tol=1e-04,
            random_state=0)
y_km = km.fit_predict(X)

plt.scatter(X[y_km == 0, 0],
            X[y_km == 0, 1],
            s=50,
            c='lightgreen',
            marker='s',
            label='cluster 1')
plt.scatter(X[y_km == 1, 0],
            X[y_km == 1, 1],
            s=50,
            c='orange',
            marker='o',
            label='cluster 2')
plt.scatter(X[y_km == 2, 0],
            X[y_km == 2, 1],
            s=50,
            c='lightblue',
            marker='v',
            label='cluster 3')
plt.scatter(km.cluster_centers_[:, 0],
            km.cluster_centers_[:, 1],
            s=250,
            marker='*',
            c='red',
            label='centroids')
plt.legend()
plt.tight_layout()
plt.show()
```

```
C:\Users\wangf\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1382: UserWarning: KMeans is known to hav
e a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by set
ting the environment variable OMP_NUM_THREADS=1.
  warnings.warn(
```



Clustering: K-means Algorithm

- Solving this problem in an **optimal** way is an **NP-Hard** problem
- A **non-optimal solution** to this problem can be obtained with **K-means algorithm.**
- In practice, K-means plus other heuristics make the approach usable in multiple problems.

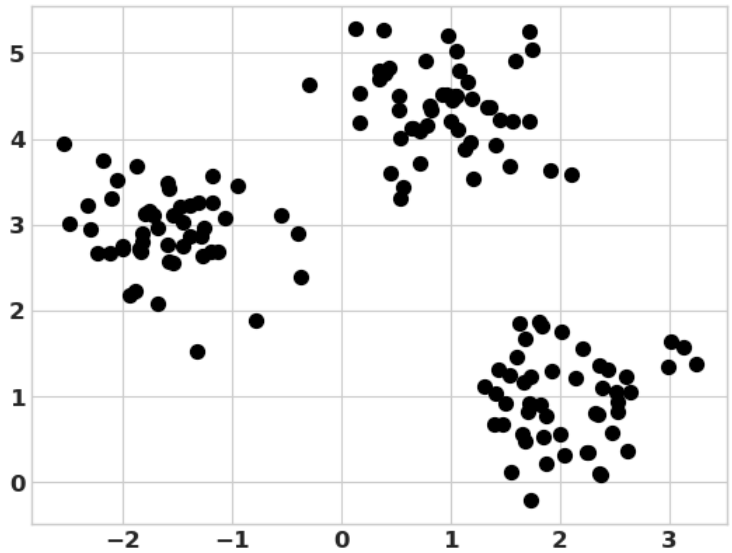
Remember that we have to find:

1. A set of points **"centroids"** $\{\mu_1, \ldots, \mu_k\}$ where $\mu \in \mathrm{R}^d$,
2. A list of **assignment labels** that create a **mapping from data points to centroids** $\{y_1, \ldots, y_n\}$

Let's think how we can solve it

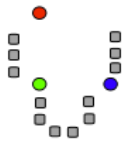
What would you do?

In [9]:
```
plt.scatter(X[:, 0], X[:, 1], c='black', marker='o', s=50)
plt.show()
```



1. We need some "reference" centroids to start

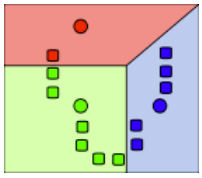
- **Initialization:** Random sample the K centroids $\{\mu_1, \ldots, \mu_k\}$
- A trick is using available points (just choose a few of them)



Figures Credit

2. Assignment Step

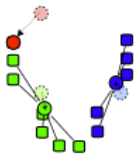
- For every point $i = [1, \ldots, N]$ compute the assignment wrt to the K clusters.
  - We have to compare $N \times K$ points (`#data points x #clusters`)
  - Given a point $\mathbf{x}_i$, **we have to find the label of the "closest" centroids in $\{\mu_1, \ldots, \mu_k\}$**
    - $y_i = \arg\min_k | |\mathbf{x}_i - \mu_k| |_2^2$



- At the end of this step we should have a pair of aligned set $\{\mathbf{x}_1, \ldots, \mathbf{x_n}\}$ and $\{y_1, \ldots, y_n\}$

3. Update Step

- Now, it is the **inverse** of before. Now we consider the "centroids".
- For every centroid $k = [1, \ldots, K]$ **we update its mean based on the previous assignments:**
- Given a μ_k, we update it as $\mu_k \leftarrow \frac{\sum_i \delta\{y_i = k\}\mathbf{x}_i}{\sum_i \delta\{y_i = k\}}$



- At the end of this step we should have a pair of aligned set $\{\mathbf{x}_1, \ldots, \mathbf{x_n}\}$ and $\{y_1, \ldots, y_n\}$ and **updated centroids** $\{\mu_1, \ldots, \mu_k\}$.

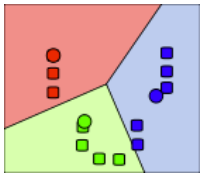
Indicator function

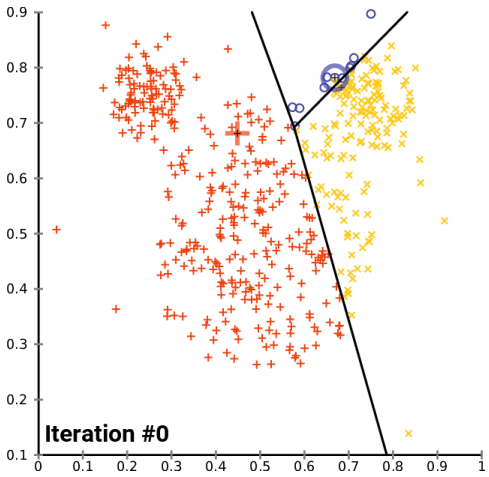
$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$$

It is a formalism to express the concept of:

- DO consider the point in the mean computation if point label corresponds to current centroid
- DO NOT consider the point in the mean computation if point label DOES NOT corresponds to current centroid

Final result





K-means (Lloyd's method)

1. **Random init of centroids**
2. Repeat until convergence:
   - **Assignment step:** $\forall i \in [1, N] \quad y_i = \arg\min_k | \, | \mathbf{x}_i - \mu_k | \, |_2^2$
   - **Update step:** $\forall k \in [1, K] \quad \mu_k \leftarrow \frac{\sum_i \delta\{y_i = k\} \mathbf{x}_i}{\sum_i \delta\{y_i = k\}}$

What does "convergence" mean?

K-means convergence

- One could check that the centroids do not change anymore (up to some ϵ), even performing more steps.
- Is there a better "convergence" term? (we will look into this later)

Let's implement a basic version with numpy

We start from this {{print(X.shape[0])}} points in {{print(X.shape[1])}}-D space

{{ plt.scatter(X[:, 0], X[:, 1], c='black', marker='o', s=50); plt.show() }}

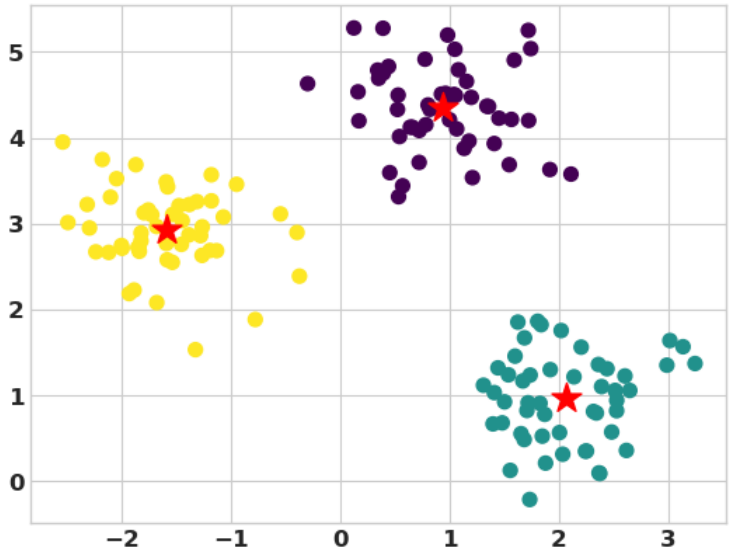
In [10]:
```python
def init(X, k):
    N, dim = X.shape
    # we select k samples from the points we have randomly
    idx = np.random.choice(N, k, replace=False)
    # the centers are just the k-random sampled points
    return X[idx]


def get_assignments(X, centers):
    P = X[:, np.newaxis, :]  # Nx1xD
    diff_sq = (P - centers)**2  # Nx1xD - KxD -> NxKxD # broadcasting
    # more info on broadcasting https://numpy.org/doc/stable/user/basics.broadcasting.html
    # dist = sum_over_axis(diff^2) then take argmin of dist across centers
    y = diff_sq.sum(axis=2).argmin(axis=1)
    return y  # Nx1 and the values inside go from [1...K]


def update_centers(X, y, K):
    # select the points to the k center and remove N dimension with mean over axis 0
    y_row = y.reshape((1, -1)) #1xN
    k_col = np.arange(K).reshape(-1, 1) #Kx1

    #M[i][j] = 1 if X[j,:] belongs to cluster i else 0
    M = k_col == y_row  #KxN

    #cluster_sum[i,:] contains the sum of all vectors in cluster i
    cluster_sum = M @ X #KxN @ NxD -> KxD

    #counts[i,:] contains the number of vectors in cluster i
    counts = np.sum(M, axis=1).reshape(-1, 1) #Kx1

    return cluster_sum / counts #KxD
```

In [11]:
```
# Double check
np.random.seed(0)  # make the method deterministic
from sklearn.metrics import pairwise_distances_argmin
centers = init(X, 3)
y_assignments = get_assignments(X, centers)
labels = pairwise_distances_argmin(X, centers)
assert np.array_equal(labels, y_assignments), 'Assignment not correct!'
```

In [12]:
```
def kmeans(X, n_clusters):
    np.random.seed(0)  # make the method deterministic
    iter = 1
    #1. init random sample the centers
    centers = init(X, n_clusters)

    while True:
        # 2. Assignment step
        y_assignments = get_assignments(X, centers)

        # 3. Update step
        new_centers = update_centers(X, y_assignments, n_clusters)

        # 4. Check for convergence
        # This is a possible implementation
        # A more formal is to check that the loss is plateauing (more on this later)
        if np.allclose(centers, new_centers):
            break
        # update cluster for next iter
        centers = new_centers

        print(f'Iteration {iter}')
        iter += 1

    return centers, y_assignments
```

In [13]:
```
centers, y_est = kmeans(X, 3)
plt.scatter(*X.T, c=y_est,
            s=50, cmap='viridis')
_ = plt.scatter(*centers.T,
                s=250,
                marker='*',
                c='red',
                label='centroids')
```

```
Iteration 1
Iteration 2
Iteration 3
```

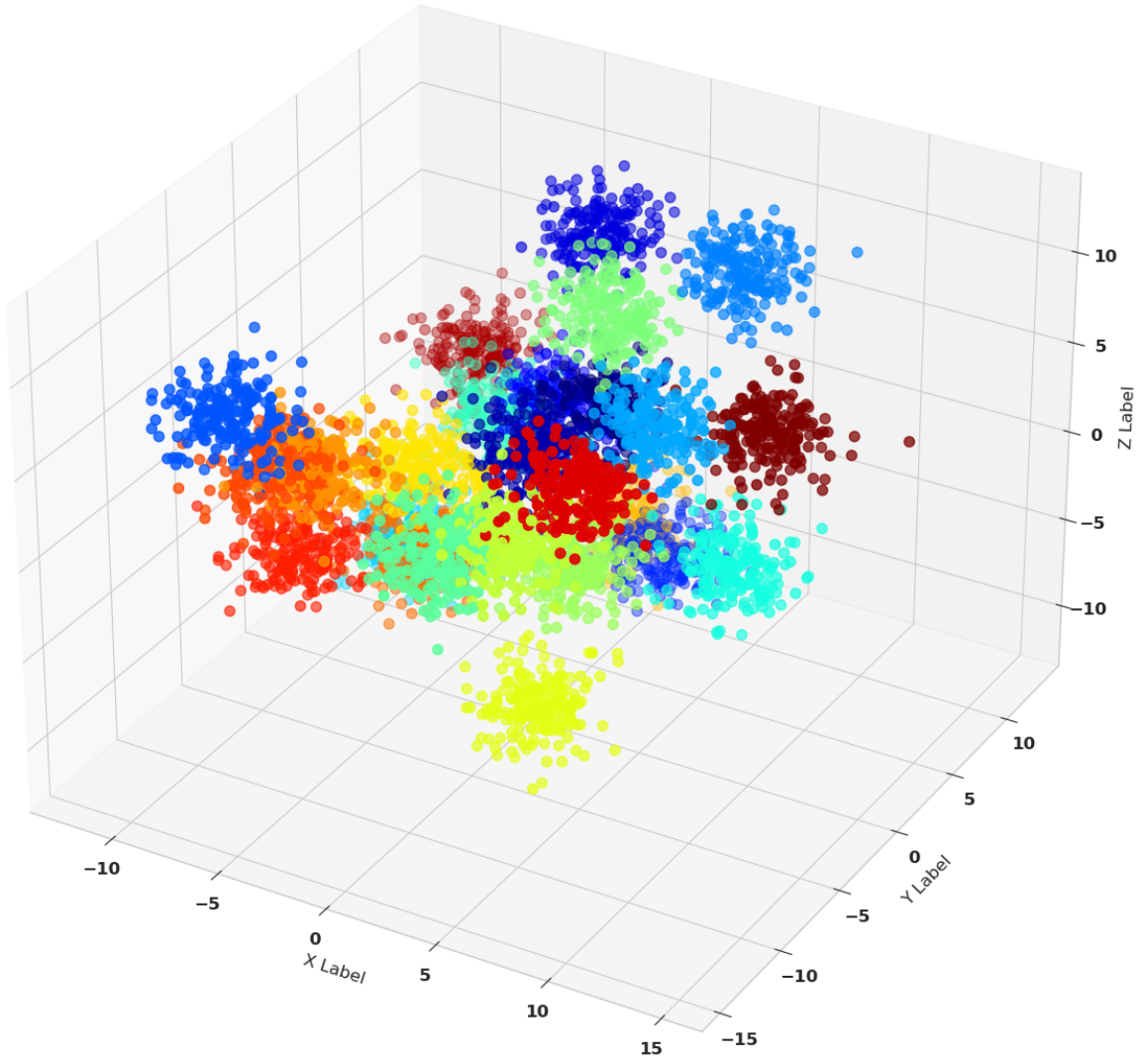


Let's try larger dataset

In [14]:
```
from sklearn.datasets import make_blobs

X, y = make_blobs(n_samples=5000,
                  n_features=3,
                  centers=25,
                  cluster_std=1.25,
                  shuffle=True,
                  random_state=0)
```

In [15]:
```
fig = plt.figure(figsize=(15,15))
ax = fig.add_subplot(projection='3d')

ax.scatter(*X.T, c=y,
           s=50, cmap='jet')

ax.set_xlabel('X Label')
ax.set_ylabel('Y Label')
_ = ax.set_zlabel('Z Label')
```

```
findfont: Font family ['Times'] not found. Falling back to DejaVu Sans.
```

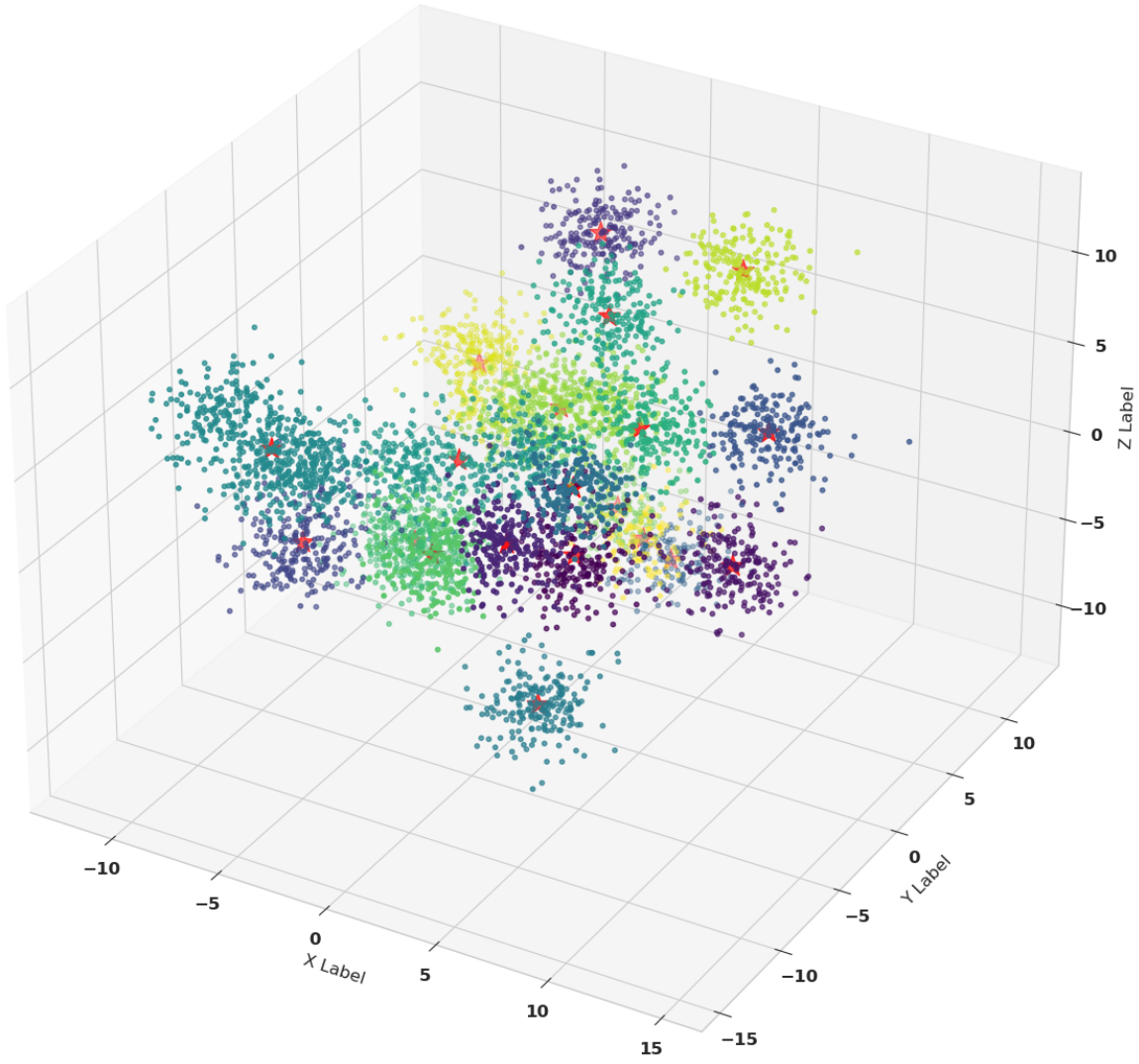


In [16]:
```
centers, y_est = kmeans(X, 20)
```

```
Iteration 1
Iteration 2
Iteration 3
Iteration 4
Iteration 5
Iteration 6
Iteration 7
Iteration 8
Iteration 9
Iteration 10
Iteration 11
Iteration 12
Iteration 13
Iteration 14
Iteration 15
Iteration 16
Iteration 17
Iteration 18
Iteration 19
Iteration 20
Iteration 21
Iteration 22
Iteration 23
Iteration 24
Iteration 25
Iteration 26
Iteration 27
Iteration 28
Iteration 29
Iteration 30
Iteration 31
Iteration 32
```

In [17]:

```
fig = plt.figure(figsize=(15,15))
ax = fig.add_subplot(projection='3d')

ax.scatter(*X.T, c=y_est,
           s=10, cmap='viridis')

ax.set_xlabel('X Label')
ax.set_ylabel('Y Label')
_ = ax.set_zlabel('Z Label')
_ = ax.scatter(*centers.T,
               s=250,
               marker='*',
               c='red',
               label='centroids')
```



Visualization

Take from this website

In [18]:

```
from sklearn.datasets import make_blobs
from sklearn.metrics import pairwise_distances_argmin

X, y_true = make_blobs(n_samples=300, centers=4,
                       cluster_std=0.60, random_state=0)

rng = np.random.RandomState(42)
centers = [0, 4] + rng.randn(4, 2)

def draw_points(ax, c, factor=1):
    ax.scatter(X[:, 0], X[:, 1], c=c, cmap='viridis',
               s=50 * factor, alpha=0.3)

def draw_centers(ax, centers, factor=1, alpha=1.0):
    ax.scatter(centers[:, 0], centers[:, 1],
               c=np.arange(4), cmap='viridis', s=200 * factor,
               alpha=alpha)
    ax.scatter(centers[:, 0], centers[:, 1],
               c='black', s=50 * factor, alpha=alpha)

def make_ax(fig, gs):
    ax = fig.add_subplot(gs)
    ax.xaxis.set_major_formatter(plt.NullFormatter())
    ax.yaxis.set_major_formatter(plt.NullFormatter())
    return ax

fig = plt.figure(figsize=(15, 4))
gs = plt.GridSpec(4, 15, left=0.02, right=0.98, bottom=0.05, top=0.95, wspace=0.2, hspace=0.2)
ax0 = make_ax(fig, gs[:4, :4])
ax0.text(0.98, 0.98, "Random Initialization", transform=ax0.transAxes,
         ha='right', va='top', size=16)
draw_points(ax0, 'gray', factor=2)
draw_centers(ax0, centers, factor=2)

for i in range(3):
    ax1 = make_ax(fig, gs[:2, 4 + 2 * i:6 + 2 * i])
    ax2 = make_ax(fig, gs[2:, 5 + 2 * i:7 + 2 * i])

    # E-step
    y_pred = pairwise_distances_argmin(X, centers)
    draw_points(ax1, y_pred)
    draw_centers(ax1, centers)

    # M-step
    new_centers = np.array([X[y_pred == i].mean(0) for i in range(4)])
    draw_points(ax2, y_pred)
    draw_centers(ax2, centers, alpha=0.3)
    draw_centers(ax2, new_centers)
    for i in range(4):
        ax2.annotate('', new_centers[i], centers[i],
                     arrowprops=dict(arrowstyle='->', linewidth=1))


    # Finish iteration
    centers = new_centers
    ax1.text(0.95, 0.95, "E-Step", transform=ax1.transAxes, ha='right', va='top', size=14)
    ax2.text(0.95, 0.95, "M-Step", transform=ax2.transAxes, ha='right', va='top', size=14)


# Final E-step
y_pred = pairwise_distances_argmin(X, centers)
axf = make_ax(fig, gs[:4, -4:])
draw_points(axf, y_pred, factor=2)
draw_centers(axf, centers, factor=2)
axf.text(0.98, 0.98, "Final Clustering", transform=axf.transAxes,
         ha='right', va='top', size=16)


fig.savefig('figs/05.11-expectation-maximization.png')
```

```
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findfont: Font family ['Times'] not found. Falling back to DejaVu Sans.
```
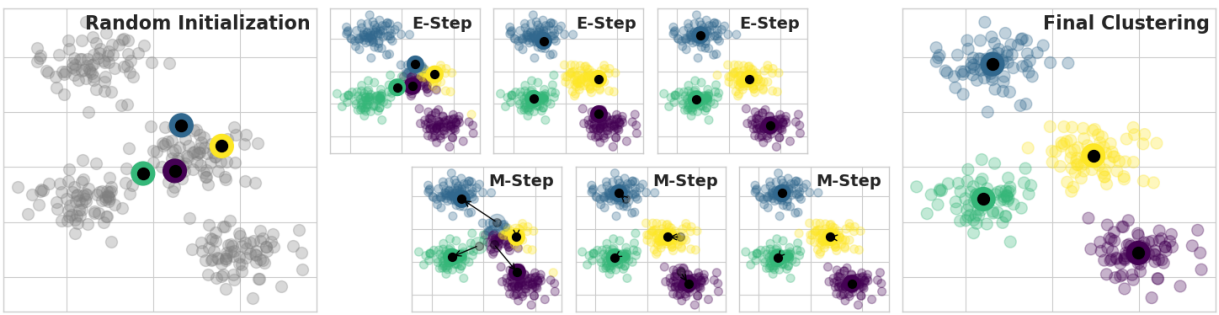
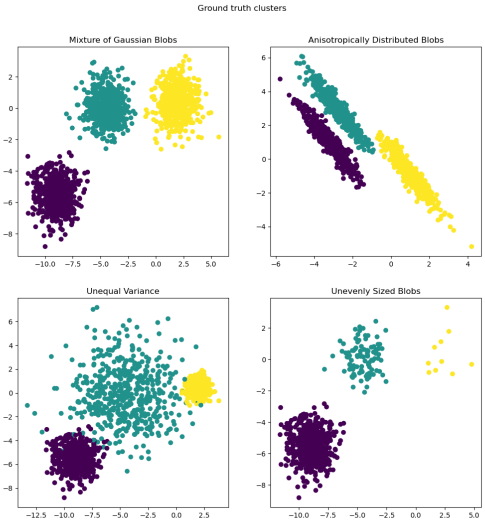



Assumptions and Limitations of K-means

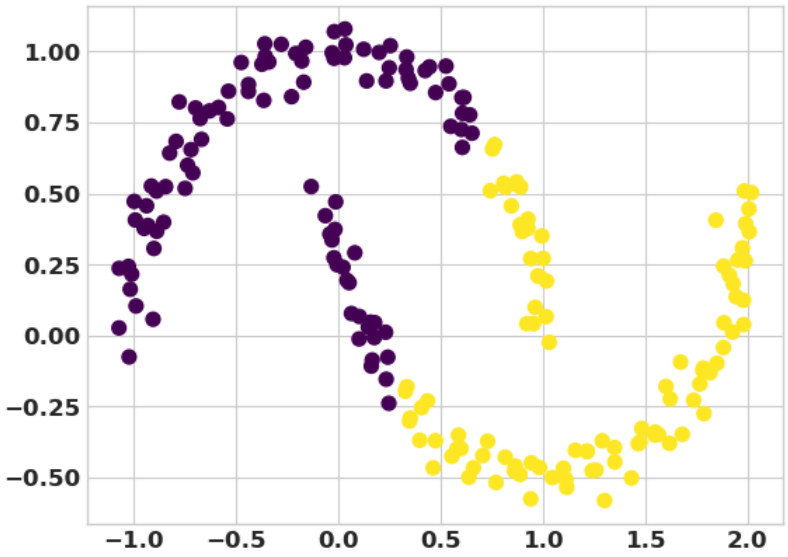
- This example is meant to illustrate situations where k-means will produce unintuitive and possibly unexpected clusters. In the first three plots, the input data does not conform to some implicit assumption that k-means makes and undesirable clusters are produced as a result.
- In the last plot, k-means returns intuitive clusters despite unevenly sized blobs.



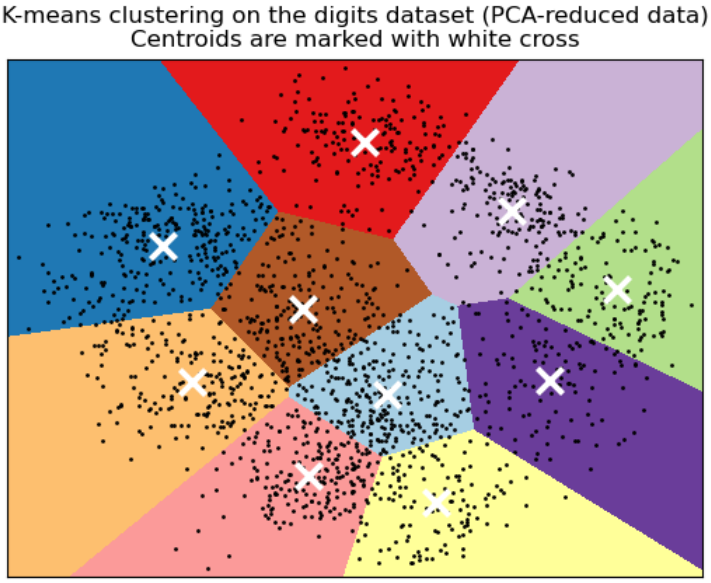
Bounded by linear cluster boundaries

In [19]:
```
from sklearn.datasets import make_moons
from sklearn.cluster import KMeans

X, y = make_moons(200, noise=.05, random_state=0)
labels = KMeans(2, random_state=0).fit_predict(X)
plt.scatter(X[:, 0], X[:, 1], c=labels,
            s=50, cmap='viridis');
```

```
C:\Users\wangf\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:870: FutureWarning: The default value of
`n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning
  warnings.warn(
C:\Users\wangf\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1382: UserWarning: KMeans is known to hav
e a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by set
ting the environment variable OMP_NUM_THREADS=1.
  warnings.warn(
```



Interpretation cluster boundaries as Voronoi Diagram

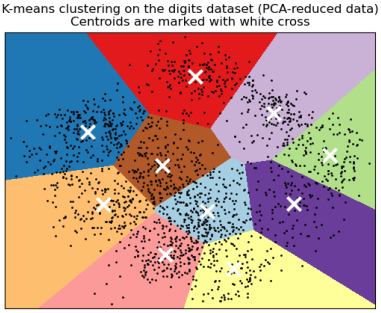


What is a Voronoi Region?

Given a set of points P_k and a distance metric $d(x, y) = \ell_2(x - y)$ and $d(x, A) = \inf \{d(x, a) \mid a \in A\}$

$$R_k = \{x \in X \mid d(x, P_k) \leq d(x, P_j) \text{ for all } j \neq k\}$$

- Points in a regions could be thought as belonging to that cluster
- Points between two regions (along a segment) are boundary points between two classes
- A point between three regions (along a single point) is boundary points between three classes



"Theory" behind K-means

- Are we guarantee that K-means will always converge? Could we be stuck in infinite loop?
- Are we reaching a global optimum in the solution?
- How much initialization matters?

K-means as a loss minimization problem

Similarly as for PCA, we can define a **loss or cost function** that can better formalize the K-means algorithm.

$$\mathrm{L}(\mu, y; \mathbf{D}) = \sum_{i=1}^{N} \left|\left| \mathbf{x}_i - \mu_{y_i} \right|\right|_2^2$$

- Criterion for separating samples in K groups of equal variance, minimizing a the "inertia" or "within-cluster sum-of-squares" (within cluster variance).
- Sum of squared distances from any data point to its assigned center

K-means as a loss minimization problem

Similarly as for PCA, we can define a **loss or cost function** that can better formalize the K-means algorithm.

$$\mathrm{L}(\mu, y; \mathbf{D}) = \sum_{i=1}^{N} \left|\left| \mathbf{x}_i - \mu_{y_i} \right|\right|_2^2 = \sum_{i=1}^{N} \min_{k \in K} \left(\left|\left| \mathbf{x}_i - \mu_k \right|\right|_2^2 \right)$$

On Convergence

- Are we guarantee that K-means will always converge? Could we be stuck in infinite loop?

> Yes, we are guarantee that K-means will always converge yet to a **LOCAL** Optimum

For any dataset **D** and any number of clusters *K*, the K-means algorithm converges in a **finite number of iterations**, where convergence is measured by the loss ceasing the change

On Convergence 👍

> For any dataset $\mathbf{D}$ and any number of clusters K, the K-means algorithm converges in a finite number of iterations, where convergence is measured by the loss L ceasing the change.

There are only two points in which the K-means algorithm changes its values.

- **Assignment step:** $\forall i \in [1, N] \quad y_i = \arg\min_k | \, | \mathbf{x}_i - \mu_k | \, |_2^2$
- **Update step:** $\forall k \in [1, K] \quad \mu_k \leftarrow \frac{\sum_i \delta\{y_i = k\} \, \mathbf{x}_i}{\sum_i \delta\{y_i = k\}}$

We will show that both of these operations can never increase the value of L. Assuming this is true, the rest of the argument is as follows.

- The possible assignments to y and μ can only take a finite number of values.
  - because y is a discrete values
  - μ is all possible means of a subset of data (it is not infinite).
  - The loss L is lower bounded by zero by ℓ_2 property.
- Together means that L cannot decrease more than a finite number of times.

It remains to show that the two steps can only decrease the loss.

1. **Assignment step:** $\forall i \in [1, N] \quad y_i = \arg\min_k | \, | \mathbf{x}_i - \mu_k | \, |_2^2$

Looking at a point i suppose that the previous value of y_i is a and the new value is b. It must be the case that $| \, | \mathbf{x}_i - \mu_b | \, |_2^2 \leq | \, | \mathbf{x}_i - \mu_a | \, |_2^2$. Thus, changing from $a \mapsto b$ **can only decrease the loss**.

- **Update step:** $\forall k \in [1, K] \quad \mu_k \leftarrow \frac{\sum_i \delta\{y_i = k\} \, \mathbf{x}_i}{\sum_i \delta\{y_i = k\}}$

Consider the second form of the loss. The update computes μ_k as the mean of the data for which $y_i = k$ which is precisely the point to minimize squared distance. So, This step too can only decrease the loss.

Practical Consideration

Though convergence is guaranteed, it does **NOT** say it is fast (i.e. it may be slow to converge for large datasets).

There are techniques such as **mini-batch K-means to speed up convergence.**

Practical implications: It will converge but to get a good results you may need either:

1. **heuristic for selecting the initial random guess** or
2. select the **best fit over multiple random initializations.**

Theoretical limitations of K-means

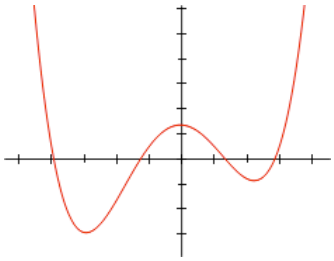
1. The convergence is only guaranteed to a **local optimum**
   - This means that with different initializations you will reach different results
   - With a global optimum, no matter where you start, if the optimization is right, you should land on the global optium (same value). **This is NOT the case of k-means.**
   - **Implication:** Initialization is important.

Theoretical limitations of K-means

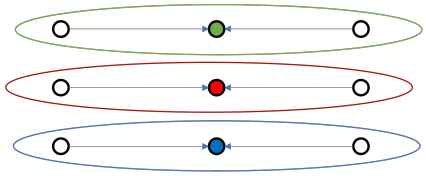
1. Second, one can show that there are input datasets and initializations on which it might take an **exponential amount of time to converge**
   - Fortunately, these cases almost never happen in practice, and in fact it has recently been shown that (roughly) if you limit the floating point precision of your machine, K-means will converge in **polynomial time** (though still only to a local optimum), using techniques of smoothed analysis.

Main problem of local optimum: Initialization

- The biggest practical issue in K-means is initialization.
- If the cluster means are initialized **poorly**, you often get convergence to uninteresting solutions.
- A useful heuristic is the **furthest-first heuristic**
- Bad Init can even happen when blobs are Gaussian and well separated
- As $k \mapsto \infty$, very **unlikely** to hit a good initialization

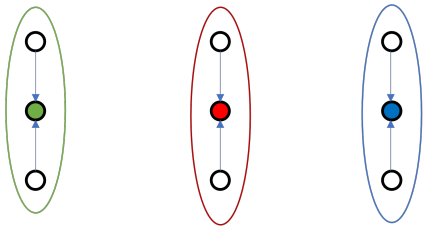


Lloyd's method (random init) can be far from global optimum



A

Which one of these configuration is best? A or B?



B

Furthest-first Heuristic

Idea: Semi-random initialization by **picking initial means as far from each other as possible**

Furthest-first Heuristic

Choose μ_1 arbitrarily between data points

- For $k = [2, \ldots, K], m = [0, \ldots, N-1]$:
  - find the data point x_m that is as far as possible from all previously selected means $[\mu_1, \ldots, \mu_{k-1}]$
  - assign $\mu_k \leftarrow x_m$

- This works well with Gaussian blobs
- but it is **sensitive to outliers**

Furthest-first Heuristic

Choose μ_1 arbitrarily between data points

- For $k = [2, \ldots, K]$:
  - $m = \arg\max_m \underbrace{\left(\min_{k<k'} \left|\left| \mathbf{x}_m - \mu_k' \right|\right|_2^2 \right)}_{\text{fix m, distance of closest centroids}}$

$\underbrace{\qquad\qquad}_{\text{select points with max distances from previous}}$

You want the point that's as far away from **all previous means as possible**

K-means++

K-mean++ paper idea is pretty "young" (from 2007)

- Do NOT take `max()` across points when selecting the centroids
- **Sample randomly but proportionally according to the distance between centroids**
- $Pr[\mu_k = \mathbf{x}_m] \propto \min_{k<k'} \left|\left| \mathbf{x}_m - \mu_k' \right|\right|_2^2$

[Arthur and Vassilvitskii 2007]

K-means++

- Note that `randomness(K-means++) > randomness(Kmeans + Furthest-first)` because with Furthest-first we select at random only at the start; then all the rest is deterministic.
- With `Kmeans++` at each cluster selection there is stochasticity involved

[Arthur and Vassilvitskii 2007]

How can we sample from a set of distances? 🤔

- Remember before we did `max(d1,...,dm)`.
- $Pr[\mu_k = \mathbf{x}_m] \propto \min_{k<k'} \left|\left| \mathbf{x}_m - \mu_k' \right|\right|_2^2$ What does this mean?

Higher distances should be more likely to get selected

In [20]:
```
dist =  np.array([1.18518298, 1.30917493, 1.10973212, 2.24523519, 1.01625606])
pmf = dist/dist.sum()
```

Inverse Transform Sampling

- Step 1. Transform the closed set D of distances into a distribution (probability mass function - pmf) as

$$p(d^{'}) = \frac{d^{'}}{\sum_{d \in D} d}$$

`dist = {{dist = np.array([1.18518298, 1.30917493, 1.10973212, 2.24523519, 1.01625606]);print(dist)}}`

to {{pmf = dist/dist.sum()}}

`pmf = {{print(pmf)}}` simply with

```
pmf = dist/dist.sum()
```

In [21]:
```
fig, axs = plt.subplots(1, 2)
fig.set_figheight(3)
fig.set_figwidth(15)
# PDF
axs[0].stem(pmf, linefmt='b-', markerfmt='bo', basefmt='--')
axs[0].set_title('PMF')
axs[0].set_xlabel('Index of distance')
axs[0].set_ylabel('Probability')
axs[0].set_aspect('auto')
# CUMSUM
axs[1].plot(np.insert(pmf.cumsum(),0,0), 'o--')
axs[1].set_title('CMF')
axs[1].set_xlabel('Index of distance')
axs[1].set_ylabel('Cumlative Probability')
axs[1].set_aspect('auto')
plt.show()
```

```
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```
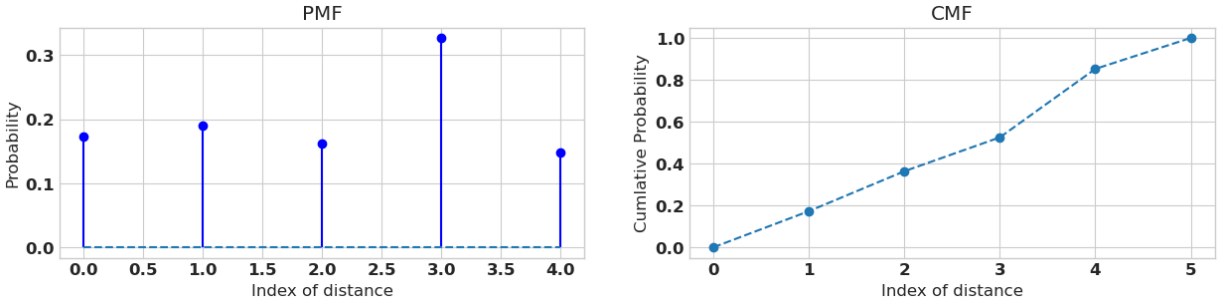
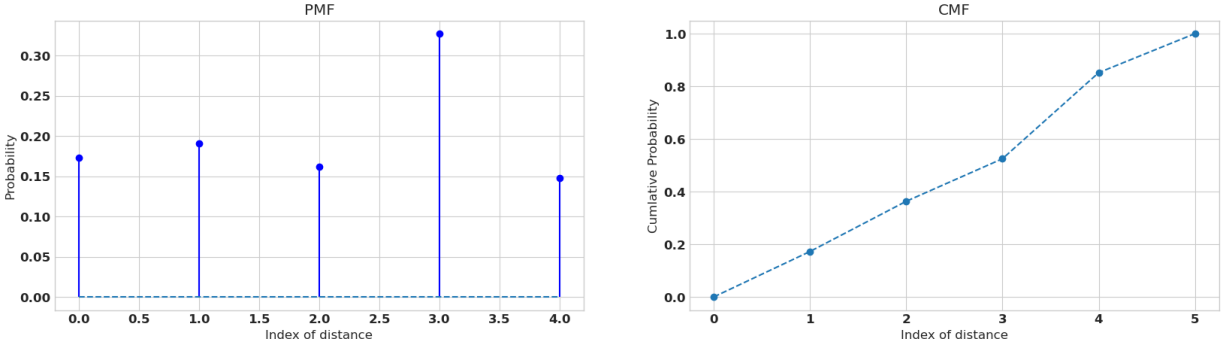



In [22]:
```
fig, axs = plt.subplots(1, 2)
fig.set_figheight(5)
fig.set_figwidth(20)
# PDF
axs[0].stem(pmf, linefmt='b-', markerfmt='bo', basefmt='--')
axs[0].set_title('PMF')
axs[0].set_xlabel('Index of distance')
axs[0].set_ylabel('Probability')
axs[0].set_aspect('auto')
# CUMSUM
axs[1].plot(np.insert(pmf.cumsum(),0,0), 'o--')
axs[1].set_title('CMF')
axs[1].set_xlabel('Index of distance')
axs[1].set_ylabel('Cumlative Probability')
axs[1].set_aspect('auto')
#axs[1].stem(pmf, linefmt='b-', markerfmt='bo', basefmt='--')
plt.show()
```



Inverse Transform Sampling for Discrete Distribution

```
U = np.random.rand(1000) #random sample uniformly from [0, 1].
# u ~ U[0,1]
# for each sampled u.
# find the first bin for which u > cumsum.
# Get the index of that bin as the sample.
sampled_idx = np.argmin((U[:, None] > pmf.cumsum()), axis=1)
```

Inverse Transform Sampling with python

```
import random
random.choices(range(0,5), weights=pmf, k=1000) #support pmf, pmf, k=how many to sample
```

Let's perform sampling and see if works

In [23]:
```
pmf.cumsum()
```

Out[23]:
```
array([0.17262675, 0.36331343, 0.52495046, 0.85197815, 1.        ])
```

In [24]:
```
U = np.array([0.13,0.25])
```

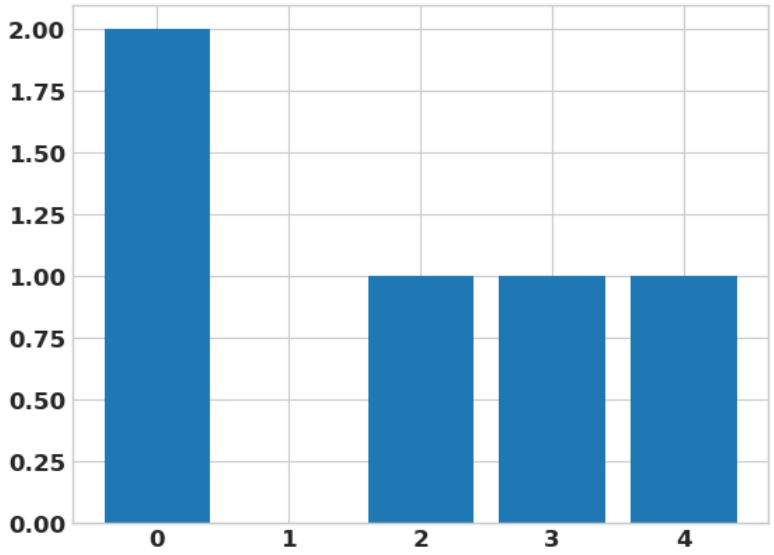
In [25]:
```
U[:, None] > pmf.cumsum()
```

Out[25]:
```
array([[False, False, False, False, False],
       [ True, False, False, False, False]])
```

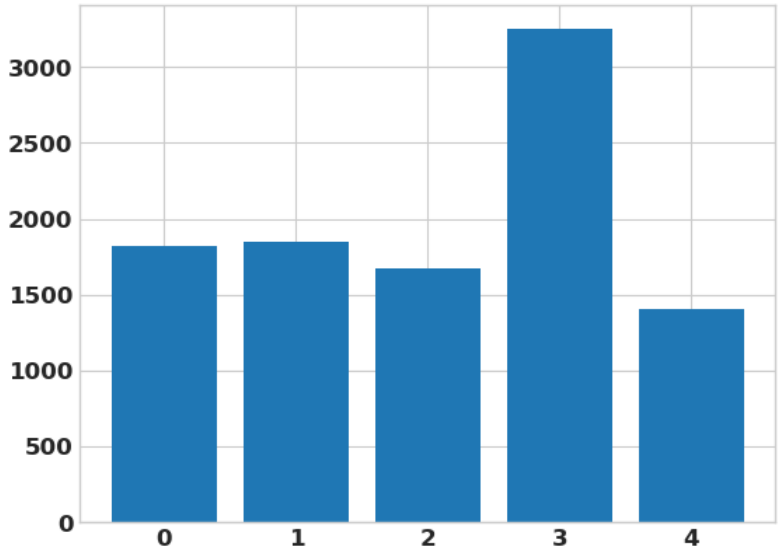
In [26]:
```
np.argmin(U[:, None] > pmf.cumsum(), axis=1)
```

Out[26]:
```
array([0, 1], dtype=int64)
```

In [27]:
```
U = np.random.rand(5)
sampled_idx = np.argmin((U[:, None] > pmf.cumsum()), axis=1)
_=plt.bar(*np.unique(sampled_idx,return_counts=True))
```



In [28]:
```
U = np.random.rand(10000)
sampled_idx = np.argmin((U[:, None] > pmf.cumsum()), axis=1)
#_ = plt.hist(sampled_idx, histtype='bar')
_=plt.bar(*np.unique(sampled_idx,return_counts=True))
```



Nice read https://stats.stackexchange.com/questions/129554/inverse-sampling-for-discrete-data

K-means++

1. Choose μ_1 arbitrarily between data points
2. For $k = [2, \ldots, K]$:
   - **Inverse Transform Sampling** wrt to distances between centroids.
   - $Pr[\mu_k = \mathbf{x}_m] \propto \min_{k<k'} \left|\left|\mathbf{x}_m - \mu_k^{'}\right|\right|_2^2$
3. Repeat until convergence Lloyd's method:
   - **Assignment step:** $\forall i \in [1, N] \quad y_i = \arg\min_k |\,|\mathbf{x}_i - \mu_k|\,|_2^2$
   - **Update step:** $\forall k \in [1, K] \quad \mu_k \leftarrow \frac{\sum_i \delta\{y_i = k\}\,\mathbf{x}_i}{\sum_i \delta\{y_i = k\}}$

K-means: a family of algorithms parametrized by the norm used

- K-means++ opens the possibility of interpret K-means as a *family* of algorithms.
- K-means++ is also called Kmeans with D^2 sampling because we sample proportionally to Euclidean norm ℓ_2.
- Interpolate between random and furthest point initialization. You can think of sampling wrt to:
  - ℓ_0 "norm" (total number of non-zero element in a vector) $\rightarrow$ random sampling
  - ℓ_2 norm $\rightarrow$ when we have K-means++
  - ℓ_∞ norm $\rightarrow$ then we have K-means with furthest-first heuristic (we take max of distances).
    - Remember our lecture on norms?

How do we choose K?

- Find a `k` that gives large gap between k-1 means and k-means cost function.
- Hold-out validation/cross-validation on auxiliary task (e.g., supervised learning task).
  - We will explain this very soon

How do we choose K?

- Simply using L as a notion of goodness is insufficient (analogous to overfitting in a supervised setting).
- A number of "information criteria" have been proposed to try to address this problem. They all effectively boil down to "regularizing" K so that the model cannot grow to be too complicated.
- The two most popular are the Bayes Information Criteria (BIC) and the Akaike Information Criteria (AIC), defined below in the context of K-means:

$$\text{(BIC)} \qquad \arg\min_K \mathrm{L}_K + \underbrace{K \cdot \log(D)}_{\text{regularization}}$$

$$\text{(AIC)} \qquad \arg\min_K \mathrm{L}_K + \underbrace{K \cdot 2D}_{\text{regularization}}$$

- Intuition is that `it is OK for the loss to go down but do not make the model (number of K) too complex`.

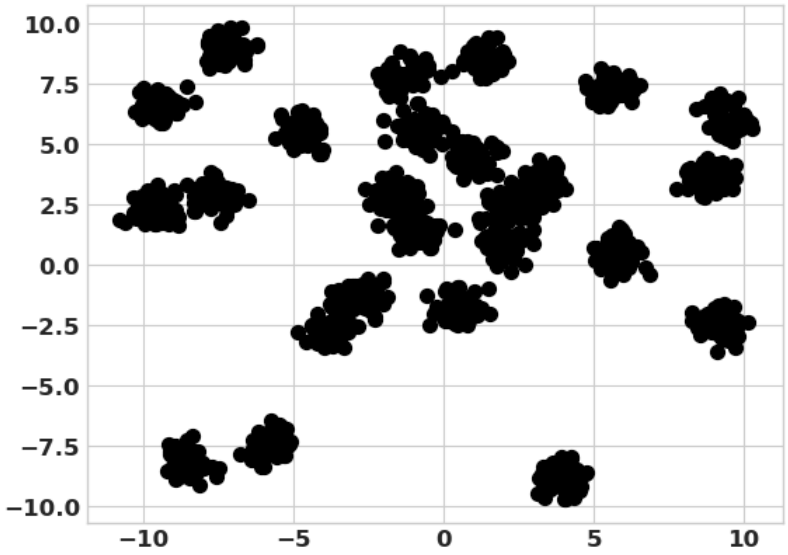
K-means Complexity

- **Initialization:** $\mathrm{O}(nd)$ One pass over data to select k centers, So $\mathrm{O}(ndk)$ time in total.
- **Lloyd's method:** $\mathrm{O}(ndk)$

- **Exponential # of rounds** in the worst case [AV07].
- Expected **polynomial time in the smoothed analysis** (non worst-case) model!
- Does well in practice

Putting all together

In [29]:
```
from sklearn.datasets import make_blobs
N_centers = 25
X, y = make_blobs(n_samples=1500,
                  n_features=2,
                  centers=N_centers,
                  cluster_std=.42,
                  shuffle=True,
                  random_state=0)

plt.scatter(X[:, 0], X[:, 1], c='black', marker='o', s=50)
plt.show()
```



In [30]:
```python
def inverse_sampling(pmf, n_samples):
    U = np.random.rand(n_samples)
    sampled_idx = np.argmin((U[:, None] > pmf.cumsum()), axis=1)
    return sampled_idx


def distance(X, centers):
    P = X[:, np.newaxis, :]  # Nx1xD
    diff_sq = (P - centers)**2  # Nx1xD - KxD -> NxKxD # broadcasting
    # more info on broadcasting https://numpy.org/doc/stable/user/basics.broadcasting.html
    # dist = sum_over_axis(diff^2) then take argmin of dist across centers
    diff_sq_sum = diff_sq.sum(axis=2)
    return diff_sq_sum


def init(X, K, plusplus=True):
    N, dim = X.shape
    if not plusplus:
        print('> Init with random sampling')
        # we select k samples from the points we have randomly
        idx = np.random.choice(N, K, replace=False)
        # the centers are just the k-random sampled points
        return X[idx]
    else:
        print('> Init with kmeans++')
        # we select a point
        idx_first = np.random.choice(N, 1)
        # init the centers and distances
        centers = X[idx_first]
        dists = distance(X, centers)
        for k in range(1, K):  # for [1.....K-1]
            # compute min across all k-centers, for all points
            # dists is NxK so min_dist is Nx1
            min_dist = dists.min(axis=1)
            # select one of the N proportional to higher distance
            idx = inverse_sampling(min_dist/min_dist.sum(), 1)
            new_center = X[idx]
            # compute distance between all points to new center
            dist_new = distance(X, new_center)
            # update pool of centers and distances
            centers = np.vstack([centers, new_center])
            dists = np.hstack([dists, dist_new])
        # the centers are computed after the loop
        return centers


def get_assignments(X, centers):
    dist_sq = distance(X, centers)  # get distance #Nxk
    y = dist_sq.argmin(axis=1)  # select argmin distance #Nx1
    return y, dist_sq.min(axis=1)  # Nx1 and the values inside go from [1...K]


def update_centers(X, y, K):
    # select the points to the k center and remove N dimension with mean over axis 0
    y_row = y.reshape((1, -1)) #1xN
    k_col = np.arange(K).reshape(-1, 1) #Kx1

    #M[i][j] = 1 if X[j,:] belongs to cluster i else 0
    M = k_col == y_row  #KxN

    #cluster_sum[i,:] contains the sum of all vectors in cluster i
    cluster_sum = M @ X #KxN @ NxD -> KxD

    #counts[i,:] contains the number of vectors in cluster i
    counts = np.sum(M, axis=1).reshape(-1, 1) #Kx1

    return cluster_sum / counts #KxD
```

In [31]:
```python
# Double check
np.random.seed(0)  # make the method deterministic
from sklearn.metrics import pairwise_distances_argmin
centers = init(X, N_centers)
y_assignments, _ = get_assignments(X, centers)
labels = pairwise_distances_argmin(X, centers)
assert np.array_equal(labels, y_assignments), 'Assignment not correct!'
```

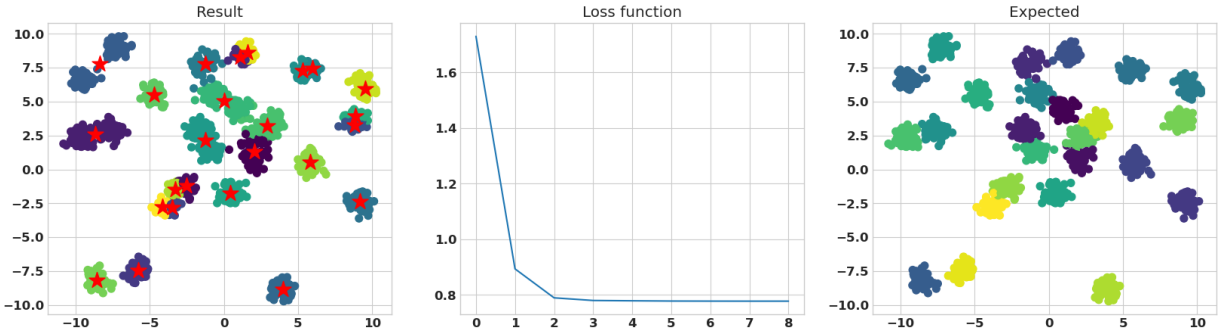
```
> Init with kmeans++
```

In [32]:
```
def kmeans(X, n_clusters):
    np.random.seed(0)  # make the method deterministic
    iter = 1
    # 1. init random sample the centers
    centers = init(X, n_clusters)
    loss = []
    while True:
        # 2. Assignment step
        y_assignments, dist_sq = get_assignments(X, centers)
        # distance between points and center, average over points
        loss.append(dist_sq.mean())
        # 3. Update step
        new_centers = update_centers(X, y_assignments, n_clusters)

        # 4. Check for convergence
        # If two last losses are close enough we stop
        if len(loss) > 2 and np.allclose(loss[-2], loss[-1], atol=1e-5):
            break
        # update cluster for next iter
        centers = new_centers

        print(f'> Iteration {iter}: loss {loss[-1]}')
        iter += 1

    return centers, y_assignments, loss
```

In [33]:
```
centers, y_est, loss = kmeans(X, N_centers)
```

```
> Init with kmeans++
> Iteration 1: loss 1.7296452170971994
> Iteration 2: loss 0.8938248433703359
> Iteration 3: loss 0.7897878328750901
> Iteration 4: loss 0.7802986159291134
> Iteration 5: loss 0.779175352001348
> Iteration 6: loss 0.778229997754058
> Iteration 7: loss 0.777968597663401
> Iteration 8: loss 0.7778315053744624
```

In [34]:
```
fig, ax = plt.subplots(1, 3, figsize=(20, 5))
ax[0].scatter(*X.T, c=y_est,
              s=50, cmap='viridis')
ax[0].set_title('Result')
_ = ax[0].scatter(*centers.T,
                  s=250,
                  marker='*',
                  c='red',
                  label='centroids')
_ = ax[1].plot(loss)
_ = ax[1].set_title('Loss function')
_ = ax[2].scatter(*X.T, c=y,
              s=50, cmap='viridis')
_ = ax[2].set_title('Expected')
```



Applications

The applications are inspired from this website

Clustering of Digits (2D images) for "classification"

In [35]:
```
from sklearn.datasets import load_digits
digits = load_digits()
digits.data.shape
```

Out[35]:
```
(1797, 64)
```

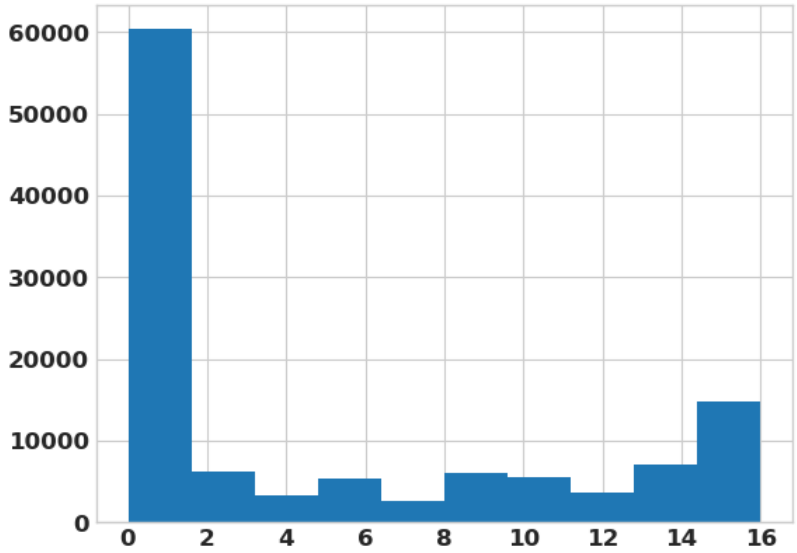
Let's see the data

- Each datapoint is a 8x8 image of a digit.

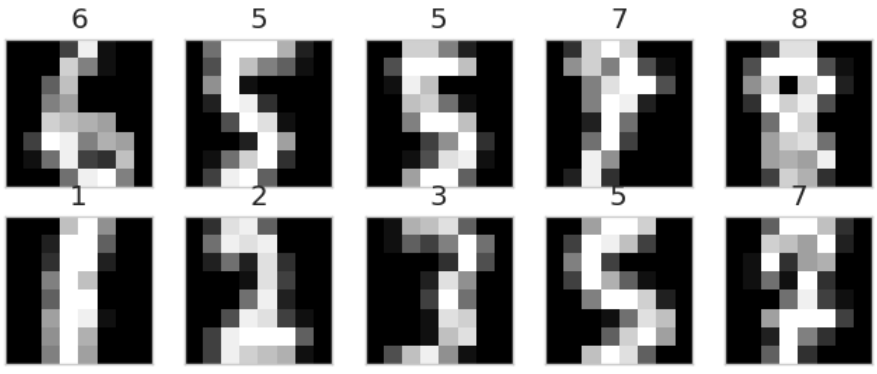
Attribute	Value
Classes	10
Samples per class	~180
Samples total	1797
Dimensionality	64
Features	int 0-15

Let's see the histogram of features (pixel colors)

In [36]:
```
_ = plt.hist(digits.data.flatten())
```

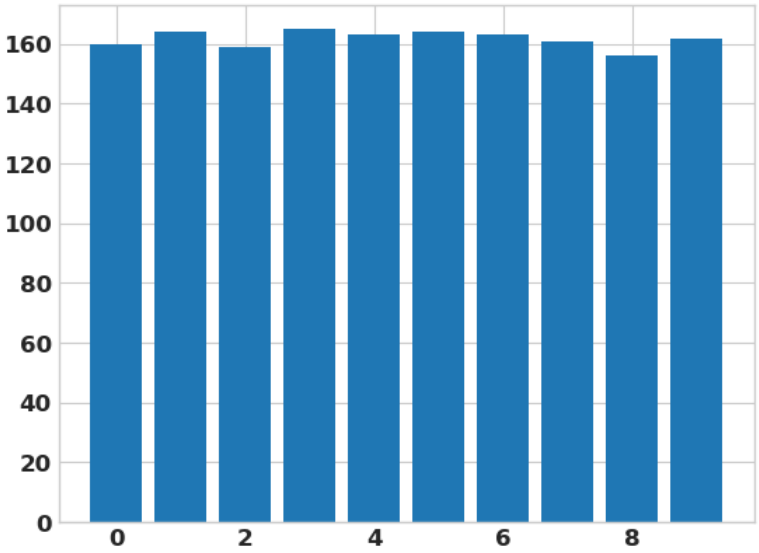


In [37]:
```
np.random.seed(13)  # fixing the seed to see same pictures

fig, ax = plt.subplots(2, 5, figsize=(8, 3))
idx = np.random.choice(digits.data.shape[0], 10)
labels = digits.target[idx, ...]
points = digits.data[idx, ...].reshape(-1, 8, 8)
for axi, vector, y in zip(ax.flat, points, labels):
    axi.set(xticks=[], yticks=[])
    axi.imshow(vector, interpolation='none', cmap='gray')
    axi.set_title(y)
```

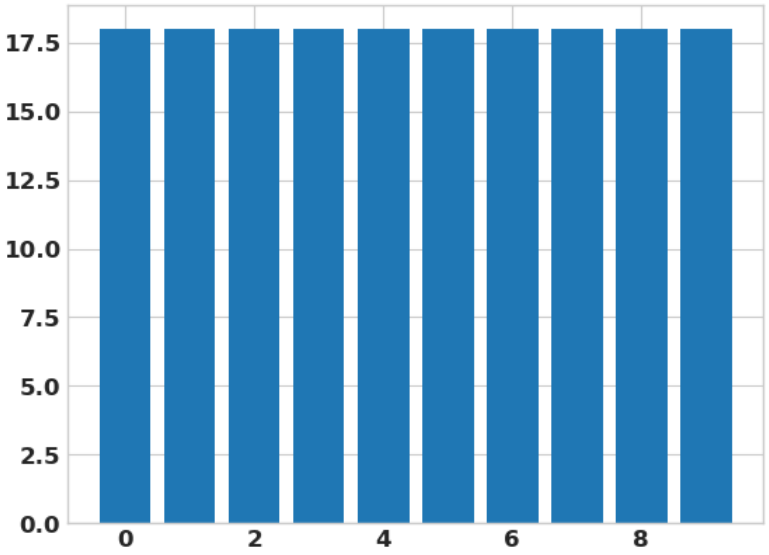


In [38]:
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(digits.data,digits.target, test_size=0.1,
                                                    random_state=0, stratify=digits.target)
```

In [39]:
```
plt.bar(*np.unique(y_train, return_counts=True));
```



In [40]:
```
plt.bar(*np.unique(y_test, return_counts=True));
```



Compute the mode from a distribution

Informally, the mode is the most frequent element

- We can count the frequency of each value
- Take the most frequent value

```
u, counts = np.unique([1,2,3,4,1,1,1,], return_counts=True)
mode = u[counts.argmax()] # will print 1 since 1 is most frequent
                          # 4 time present
```

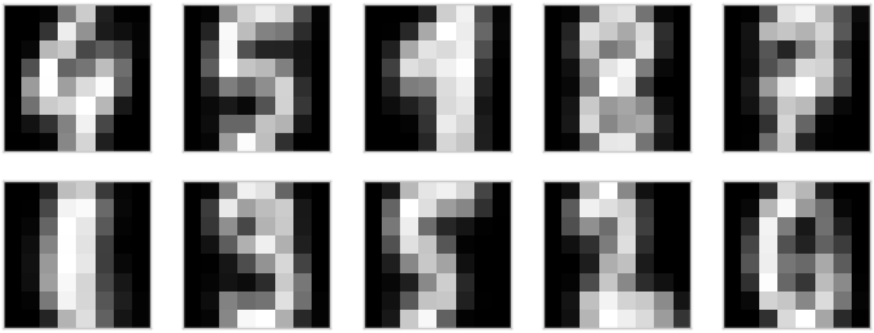
Let's run our K-means on the digits

In [41]:
```
N_centers = 10 # we assume to know that there are 10 digits
centers, y_est, loss = kmeans(X_train, N_centers)
```

```
> Init with kmeans++
> Iteration 1: loss 1314.5627705627705
> Iteration 2: loss 756.8259891509574
> Iteration 3: loss 725.4550366992323
> Iteration 4: loss 716.4499767121214
> Iteration 5: loss 711.2049934919781
> Iteration 6: loss 708.236358647983
> Iteration 7: loss 705.2994723513523
> Iteration 8: loss 701.9520972059448
> Iteration 9: loss 698.6658028658622
> Iteration 10: loss 695.5144766870222
> Iteration 11: loss 693.5266489678621
> Iteration 12: loss 692.1208906914004
> Iteration 13: loss 691.3495761746228
> Iteration 14: loss 690.657571369928
> Iteration 15: loss 690.0861205462734
> Iteration 16: loss 689.7669567135049
> Iteration 17: loss 689.6771929699328
> Iteration 18: loss 689.6572694423297
> Iteration 19: loss 689.6474580308259
> Iteration 20: loss 689.6267235993998
> Iteration 21: loss 689.6114085109643
```

Now let's visualize the centers

In [42]:
```
fig, ax = plt.subplots(2, 5, figsize=(8, 3))
centers_img = centers.reshape(10, 8, 8)
for axi, center in zip(ax.flat, centers_img):
    axi.set(xticks=[], yticks=[])
    axi.imshow(center, interpolation='none', cmap='gray')
```



It looks like a smoothed version of before...

- We see that even without the labels, `KMeans` is able to find clusters whose centers are recognizable digits, with perhaps the exception of 1 and 8.
- Probably in this case, the dataset is "easy" and distances among points have a lot of informations.

- Because k-means knows nothing about the identity of the cluster, the 0–9 labels may be permuted.
  - We can fix this by matching each learned cluster label with the true labels found in them
  - In this step we are only computing the mapping between each "color" that kmeans assign to the cluster to each digit label
  - We **CANNOT** change the assignment to each cluster. This is meant just to map "colors" to actual digit labels.

In [43]:
```
def get_mode(X):
    values, counts = np.unique(X, return_counts=True)
    return values[counts.argmax()]

# Nx1
labels = np.zeros_like(y_est)
# 10x1
center_label = np.zeros((N_centers), dtype=np.int32)

for i in range(N_centers):
    mask = (y_est == i)
    mode_y = get_mode(y_train[mask])
    labels[mask] = mode_y
    center_label[i] = mode_y
```

In [44]:
```
from sklearn.metrics import accuracy_score
accuracy_score(y_train, labels)
```

Out[44]:
```
0.7043908472479901
```

Not bad at accuracy of ~70% just with unsupervised method on the "training set" though no label has been used for training

Remember: Random chance accuracy over 10 classes is 1/10 ~10%.

We also have validated our implementation of K-means

Further, There is hope this may translate to test set

In [45]:
```
# sum over axis of dimensionality of squared difference
# Nx1x64 vs 10x64 --> Nx10x64 --sum axis 2 ---> Nx10
# we match the test wrt to the center (there might be other classification methods)
L2_square = ((X_test[...,np.newaxis,:] - centers)**2).sum(axis=2)
```

In [46]:
```
# Nx10 -- argmin over axis --> Nx1
idx_cluster = L2_square.argmin(axis=1)
```

In [47]:
```
y_test_estimated = center_label[idx_cluster]
```

In [48]:
```
accuracy_score(y_test, y_test_estimated)
```

Out[48]:
```
0.6722222222222223
```

Not bad at accuracy of ~67% just with unsupervised method on the "test split"

Remember: Random chance accuracy over 10 classes is 1/10 ~10%

Note now things are easy because:

1. `digits` is an easy dataset. Which means distance in the pixel-space contains useful informations.
2. In real-world unsupervised learning does not work so well.

It is OK to implement things manually in a course but remember that you can use optimized implementation via sklearn.

```
from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=4)
kmeans.fit(X)
y_kmeans = kmeans.predict(X)
```

Homework 1a: Repeat the experiments but not project the data onto a lower dimensional subspace and retain 99% of the variance. Does the classification improve? [WITHOUT sklearn, rewriting all code without looking at this; for each line of code write the matrix shape to validate your implementation]

Note: I did not try so I do not know what happens, but you can make hypothesis. Before running it, make an hypothesis of what is going to happen following a rationale in your mind, based on what we studied so far. Then after formulating the hypothesis, do the experiments.

Tips 1: Try to retain all the features (i.e. 100% of variance) in case accuracy does not improve. In this case you are just rotating the data and decorrelating the covariance matrix

Tips 2: If you try multiple runs, remember to FIX THE RANDOM SEED to make the experiments comparable

Homework 1b: To debug what happens, you can plot the data in 2D or 3D with PCA and show the digits ID with a color using a colormap

Homework 1c *[Advanced]*: To visualize the digits dataset, now use an advanced dimensionality reduction algorithm called `t-SNE`. Unlike PCA this method supports, multiple non-linear structures so you should see the digits more separated in 2D. For this use sklearn!

Homework 2: Repeat everything but now use sklearn.

Color Compression with K-means

In [49]:
```
# Note: this requires the ``pillow`` package to be installed
from sklearn.datasets import load_sample_image
china = load_sample_image("china.jpg")
fig, ax = plt.subplots(1, 1, figsize=(20, 15))
ax.set(xticks=[], yticks=[])
ax.imshow(china)
```

Out[49]:
```
<matplotlib.image.AxesImage at 0x18a501596d0>
```

In [50]:
```
# Note: this requires the ``pillow`` package to be installed
from sklearn.datasets import load_sample_image
china = load_sample_image("china.jpg")
fig, ax = plt.subplots(1, 1, figsize=(20, 15))
ax.set(xticks=[], yticks=[])
ax.imshow(china)
```

Out[50]:
```
<matplotlib.image.AxesImage at 0x18a5019d0d0>
```

- This is a {{china.shape}} image `WxHx3` where 3 is RGB but can also be seen as a 3D point cloud.
- Each pixel is a point in 3D where 3 dimensions are R, G, B

Let's normalize the data to stay in 3D hypercube of length 1

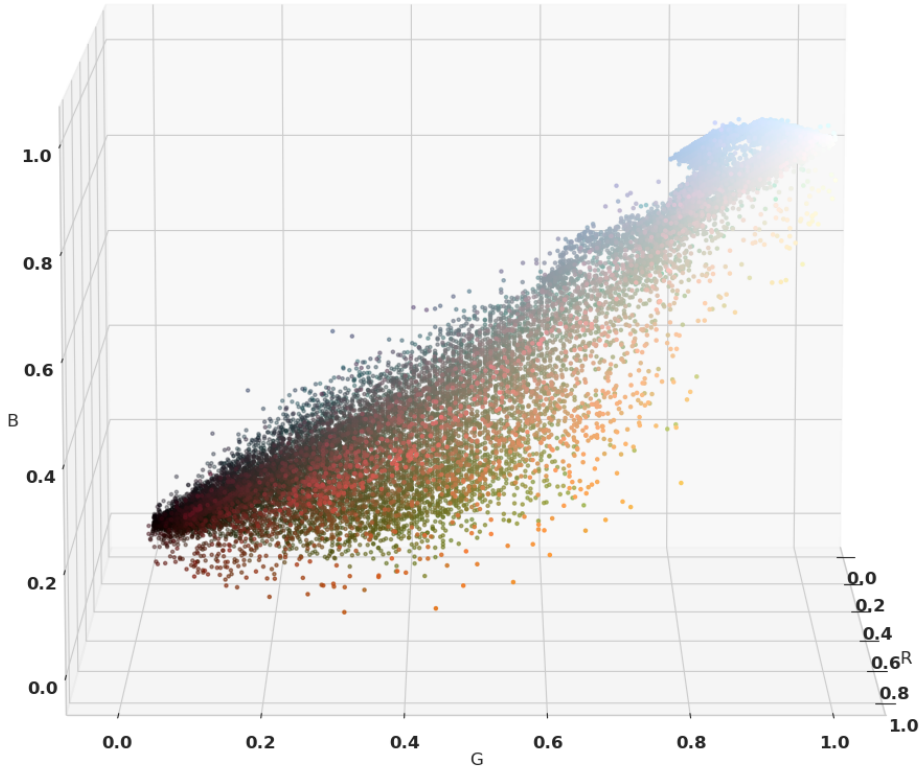
```
data = china/255.0 # scale all points to 0...1
data = data.reshape(-1,3)
```

In [51]:
```
data = china/255.0 # scale all points to 0...1
data = data.reshape(-1,3)
data.shape
```

Out[51]:
```
(273280, 3)
```

The 3D point cloud

In [52]:
```
fig = plt.figure(figsize=(15,15))
ax = fig.add_subplot(projection='3d')
data_sampled = data[::10] #1 point every 10 to go faster
ax.scatter(*data_sampled.T, marker='.', color=data_sampled)
ax.set_xlabel('R')
ax.set_ylabel('G')
_ = ax.set_zlabel('B')
ax.view_init(elev=10, azim=(0))
```



How many possible points in this 3D cube?

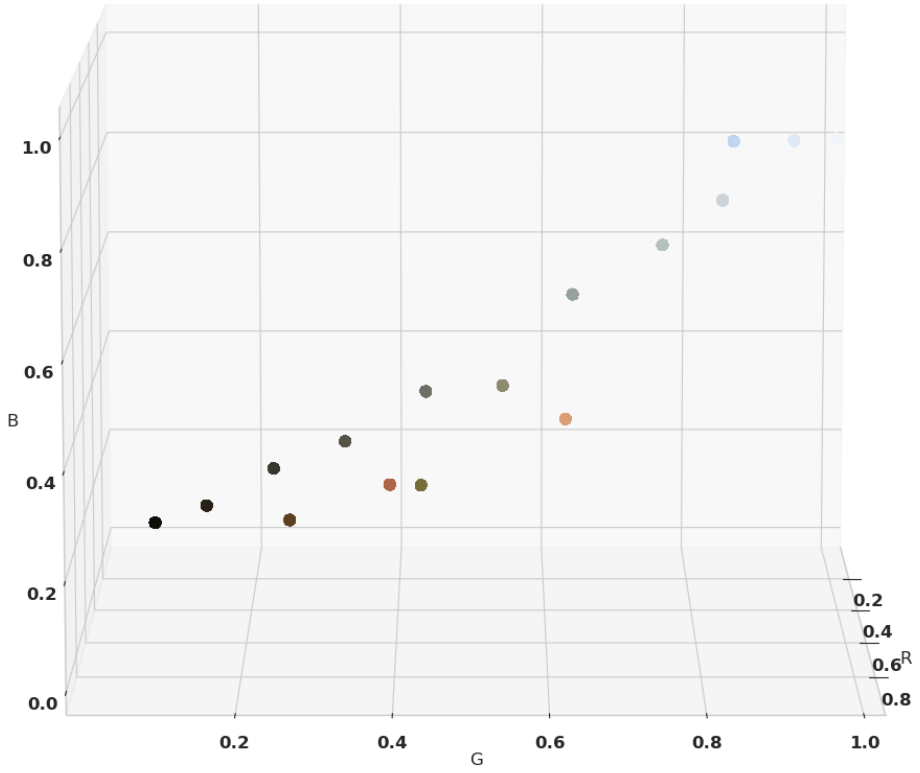
$256^3 \approx 16$ millions

Now we quantize the colors with K-means to 16 colors

In [53]:
```
from sklearn.cluster import KMeans
kmeans = KMeans(16)
kmeans.fit(data)
y_est = kmeans.predict(data) # predict cluster center (project)
new_colors = kmeans.cluster_centers_[y_est] # backproject to the colors centers
```

```
C:\Users\wangf\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:870: FutureWarning: The default value of
`n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning
  warnings.warn(
```

In [54]:
```
fig = plt.figure(figsize=(15, 15))
ax = fig.add_subplot(projection='3d')
data_sampled = new_colors[::10]  # 1 point every 10 to go faster
ax.scatter(*data_sampled.T, marker='.', color=data_sampled, s=200)
ax.set_xlabel('R')
ax.set_ylabel('G')
_ = ax.set_zlabel('B')
ax.view_init(elev=10, azim=(0))
```



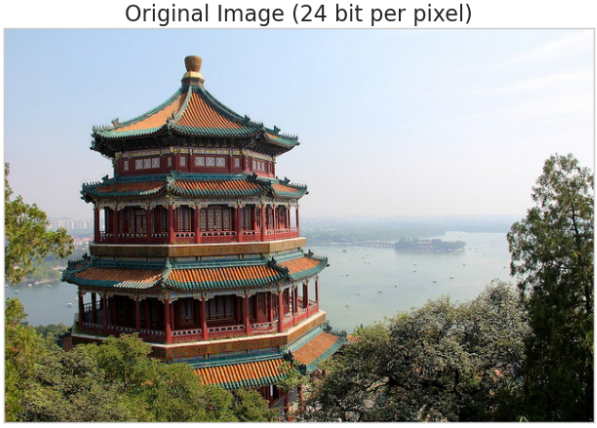
Note

- **Important:** new_colors has the same shape of original images but inside the colors get "quantized" into 16 possible colors (the k-means centers)

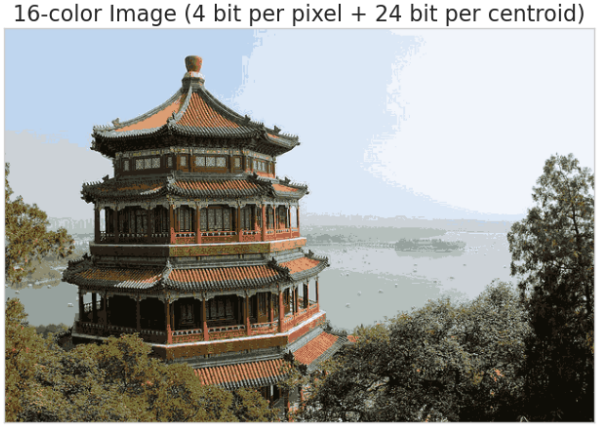
In [55]:
```
china_recolored = new_colors.reshape(china.shape)

fig, ax = plt.subplots(1, 2, figsize=(16, 6),
                       subplot_kw=dict(xticks=[], yticks=[]))
fig.subplots_adjust(wspace=0.05)
ax[0].imshow(china)
ax[0].set_title('Original Image (24 bit per pixel)', size=16) # 8 bit per channel, for each pixel
ax[1].imshow(china_recolored)
ax[1].set_title('16-color Image (4 bit per pixel + 24 bit per centroid)', size=16);
```

```
findfont: Font family ['Times'] not found. Falling back to DejaVu Sans.
```

Original Image (24 bit per pixel)



16-color Image (4 bit per pixel + 24 bit per centroid)



Bag of Visual Words: how to construct an image recogntion pipeline

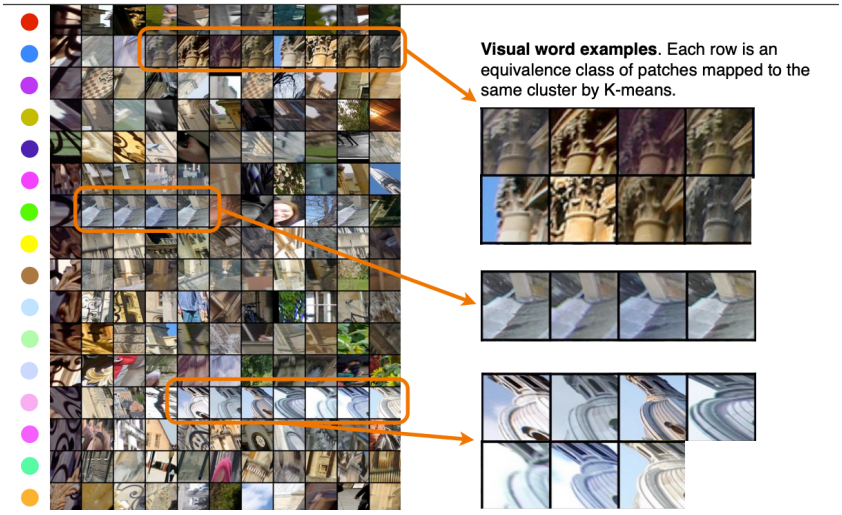


Figure Credit Prof. Vedaldi - Oxford

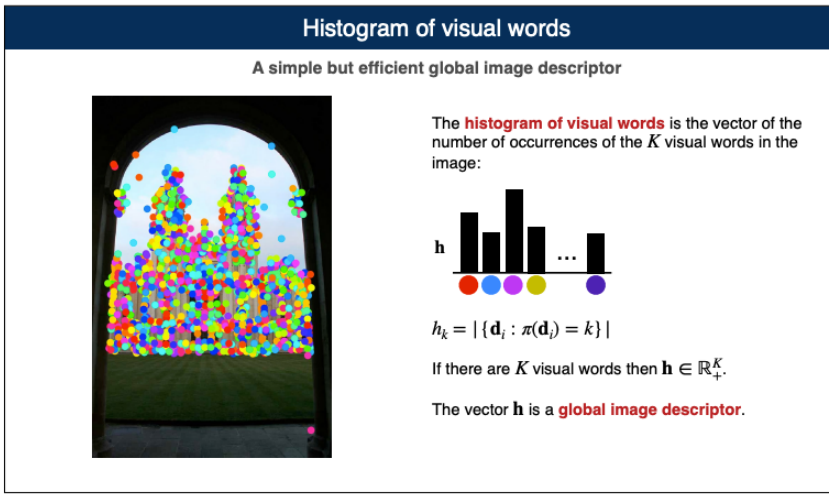


Figure Credit Prof. Vedaldi - Oxford