

Exercise

12

TUM Department of Informatics

Supervised by	Prof. Dr. Stephan Günnemann Informatics 3 - Professorship of Data Mining and Analytics
Submitted by	Marcel Bruckner (03674122) Julian Hohenadel (03673879) Kevin Bein (03707775)
Submission date	Munich, February 2, 2020

Dimensionality Reduction & Clustering

Problem 1:

exercise_12_matrix_factorization

February 2, 2020

0.1 Exporting the results to PDF

Once you complete the assignments, export the entire notebook as PDF and attach it to your homework solutions. The best way of doing that is 1. Run all the cells of the notebook. 2. Export/download the notebook as PDF (File -> Download as -> PDF via LaTeX (.pdf)). 3. Concatenate your solutions for other tasks with the output of Step 2. On linux, you can use `pdffunite`, there are similar tools for other platforms, too. You can only upload a single PDF file to Moodle.

Make sure you are using `nbconvert` version 5.5 or later by running `jupyter nbconvert --version`. Older versions clip lines that exceed page width, which makes your code harder to grade.

1 Matrix Factorization

```
In [1]: import time
import scipy.sparse as sp
import numpy as np
from scipy.sparse.linalg import svds
from sklearn.linear_model import Ridge

import matplotlib.pyplot as plt
%matplotlib inline
```

1.1 Restaurant recommendation

The goal of this task is to recommend restaurants to users based on the rating data in the Yelp dataset. For this, we try to predict the rating a user will give to a restaurant they have not yet rated based on a latent factor model.

Specifically, the objective function (loss) we wanted to optimize is:

$$\mathcal{L} = \min_{P,Q} \sum_{(i,x) \in W} (M_{ix} - \mathbf{q}_i^T \mathbf{p}_x)^2 + \lambda \sum_x \|\mathbf{p}_x\|^2 + \lambda \sum_i \|\mathbf{q}_i\|^2$$

where W is the set of (i, x) pairs for which the rating M_{ix} given by user i to restaurant x is known. Here we have also introduced two regularization terms to help us with overfitting where λ is hyper-parameter that control the strength of the regularization.

Hint 1: Using the closed form solution for regression might lead to singular values. To avoid this issue perform the regression step with an existing package such as `scikit-learn`. It is advisable to use ridge regression to account for regularization.

Hint 2: If you are using the scikit-learn package remember to set `fit_intercept = False` to only learn the coefficients of the linear regression.

1.1.1 Load and Preprocess the Data (nothing to do here)

```
In [2]: ratings = np.load("exercise_12_matrix_factorization_ratings.npy")
```

```
In [3]: # We have triplets of (user, restaurant, rating).
        ratings
```

```
Out[3]: array([[101968,   1880,    1],
               [101968,    284,    5],
               [101968,   1378,    2],
               ...,
               [ 72452,   2100,    4],
               [ 72452,   2050,    5],
               [ 74861,   3979,    5]], dtype=int64)
```

Now we transform the data into a matrix of dimension $[N, D]$, where N is the number of users and D is the number of restaurants in the dataset. We store the data as a sparse matrix to avoid out-of-memory issues.

```
In [4]: n_users = np.max(ratings[:,0] + 1)
        n_restaurants = np.max(ratings[:,1] + 1)
        M = sp.coo_matrix((ratings[:,2], (ratings[:,0], ratings[:,1])), shape=(n_users, n_restaurants))
        M
```

```
Out[4]: <337867x5899 sparse matrix of type '<class 'numpy.int64'>'
        with 929606 stored elements in Compressed Sparse Row format>
```

To avoid the cold start problem, in the preprocessing step, we recursively remove all users and restaurants with 10 or less ratings.

Then, we randomly select 200 data points for the validation and test sets, respectively.

After this, we subtract the mean rating for each users to account for this global effect.

Note: Some entries might become zero in this process -- but these entries are different than the 'unknown' zeros in the matrix. We store the indices for which we the rating data available in a separate variable.

```
In [5]: def cold_start_preprocessing(matrix, min_entries):
        """
        Recursively removes rows and columns from the input matrix which have less than min_entries ratings.

        Parameters
        -----
        matrix      : sp.spmatrix, shape [N, D]
                     The input matrix to be preprocessed.
        min_entries : int
                     Minimum number of nonzero elements per row and column.
```

```

Returns
-----
matrix      : sp.spmatrix, shape [N', D']
                The pre-processed matrix, where N' <= N and D' <= D

"""
print("Shape before: {}".format(matrix.shape))

shape = (-1, -1)
while matrix.shape != shape:
    shape = matrix.shape
    nnz = matrix>0
    row_ixs = nnz.sum(1).A1 > min_entries
    matrix = matrix[row_ixs]
    nnz = matrix>0
    col_ixs = nnz.sum(0).A1 > min_entries
    matrix = matrix[:,col_ixs]
print("Shape after: {}".format(matrix.shape))
nnz = matrix>0
assert (nnz.sum(0).A1 > min_entries).all()
assert (nnz.sum(1).A1 > min_entries).all()
return matrix

```

1.1.2 Task 1: Implement a function that subtracts the mean user rating from the sparse rating matrix

```

In [6]: def shift_user_mean(matrix):
        """
        Subtract the mean rating per user from the non-zero elements in the input matrix.

        Parameters
        -----
        matrix : sp.spmatrix, shape [N, D]
                Input sparse matrix.

        Returns
        -----
        matrix : sp.spmatrix, shape [N, D]
                The modified input matrix.

        user_means : np.array, shape [N, 1]
                    The mean rating per user that can be used to recover the absolute rat

        """

        # TODO: Compute the modified matrix and user_means
        non_zeros = (matrix>0)
        user_means = matrix.sum(1) / non_zeros.sum(1)
        matrix -= sp.csr_matrix(user_means).multiply(non_zeros)

```

```

assert np.all(np.isclose(matrix.mean(1), 0))
return matrix, user_means

```

1.1.3 Split the data into a train, validation and test set (nothing to do here)

```

In [7]: def split_data(matrix, n_validation, n_test):
        """
        Extract validation and test entries from the input matrix.

        Parameters
        -----
        matrix          : sp.spmatrix, shape [N, D]
                        The input data matrix.
        n_validation     : int
                        The number of validation entries to extract.
        n_test          : int
                        The number of test entries to extract.

        Returns
        -----
        matrix_split    : sp.spmatrix, shape [N, D]
                        A copy of the input matrix in which the validation and test entries are zeroed out.
        val_idx         : tuple, shape [2, n_validation]
                        The indices of the validation entries.
        test_idx        : tuple, shape [2, n_test]
                        The indices of the test entries.
        val_values       : np.array, shape [n_validation, ]
                        The values of the input matrix at the validation indices.
        test_values     : np.array, shape [n_test, ]
                        The values of the input matrix at the test indices.

        """

        matrix_cp = matrix.copy()
        non_zero_idx = np.argwhere(matrix_cp)
        ix = np.random.permutation(non_zero_idx)
        val_idx = tuple(ix[:n_validation].T)
        test_idx = tuple(ix[n_validation:n_validation + n_test].T)

        val_values = matrix_cp[val_idx].A1
        test_values = matrix_cp[test_idx].A1

        matrix_cp[val_idx] = matrix_cp[test_idx] = 0

```

```

        matrix_cp.eliminate_zeros()

    return matrix_cp, val_idx, test_idx, val_values, test_values

In [8]: M = cold_start_preprocessing(M, 20)

Shape before: (337867, 5899)
Shape after: (3529, 2072)

In [9]: n_validation = 200
        n_test = 200
        # Split data
        M_train, val_idx, test_idx, val_values, test_values = split_data(M, n_validation, n_test)

In [10]: # Remove user means.
        nonzero_indices = np.argwhere(M_train)
        M_shifted, user_means = shift_user_mean(M_train)
        # Apply the same shift to the validation and test data.
        val_values_shifted = val_values - user_means[np.array(val_idx).T[:,0]].A1
        test_values_shifted = test_values - user_means[np.array(test_idx).T[:,0]].A1

```

1.1.4 Compute the loss function (nothing to do here)

```

In [11]: def loss(values, ix, Q, P, reg_lambda):
        """
        Compute the loss of the latent factor model (at indices ix).
        Parameters
        -----
        values : np.array, shape [n_ixs,]
            The array with the ground-truth values.
        ix : tuple, shape [2, n_ixs]
            The indices at which we want to evaluate the loss (usually the nonzero indices).
        Q : np.array, shape [N, k]
            The matrix Q of a latent factor model.
        P : np.array, shape [k, D]
            The matrix P of a latent factor model.
        reg_lambda : float
            The regularization strength

        Returns
        -----
        loss : float
            The loss of the latent factor model.

        """
        mean_sse_loss = np.sum((values - Q.dot(P)[ix])**2)
        regularization_loss = reg_lambda * (np.sum(np.linalg.norm(P, axis=0)**2) + np.sum(np.linalg.norm(Q, axis=0)**2))

        return mean_sse_loss + regularization_loss

```

1.2 Alternating optimization

In the first step, we will approach the problem via alternating optimization, as learned in the lecture. That is, during each iteration you first update Q while having P fixed and then vice versa.

1.2.1 Task 2: Implement a function that initializes the latent factors Q and P

```
In [12]: def initialize_Q_P(matrix, k, init='random'):
        """
        Initialize the matrices  $Q$  and  $P$  for a latent factor model.

        Parameters
        -----
        matrix : sp.spmatrix, shape [N, D]
                The matrix to be factorized.
        k       : int
                The number of latent dimensions.
        init    : str in ['svd', 'random'], default: 'random'
                The initialization strategy. 'svd' means that we use SVD to initialize  $P$ 
                the entries in  $P$  and  $Q$  randomly in the interval  $[0, 1)$ .

        Returns
        -----
        Q : np.array, shape [N, k]
            The initialized matrix  $Q$  of a latent factor model.

        P : np.array, shape [k, D]
            The initialized matrix  $P$  of a latent factor model.
        """
        np.random.seed(0)

        N, D = matrix.shape
        if init == 'svd':
            U, s, V = svds(matrix, k=k)
            S = np.diag(s)
            Q = U.dot(S)
            P = V
        else:
            Q = np.random.random((N, k))
            P = np.random.random((k, D))

        assert Q.shape == (matrix.shape[0], k)
        assert P.shape == (k, matrix.shape[1])
        return Q, P
```

1.2.2 Task 3: Implement the alternating optimization approach

```
In [15]: def latent_factor_alternating_optimization(M, non_zero_idx, k, val_idx, val_values,
            reg_lambda, max_steps=100, init='random',
```



```

log_every=1, patience=5, eval_every=1):
"""
Perform matrix factorization using alternating optimization. Training is done via
i.e. we stop training after we observe no improvement on the validation loss for
amount of training steps. We then return the best values for Q and P observed during
training.

Parameters
-----
M
    : sp.spmatrix, shape [N, D]
    The input matrix to be factorized.

non_zero_idx
    : np.array, shape [nnz, 2]
    The indices of the non-zero entries of the un-shifted matrix.
    nnz refers to the number of non-zero entries. Note that this is not the same as
    from the number of non-zero entries in the input matrix M, e.g. if a user has
    that all ratings by a user have the same value.

k
    : int
    The latent factor dimension.

val_idx
    : tuple, shape [2, n_validation]
    Tuple of the validation set indices.
    n_validation refers to the size of the validation set.

val_values
    : np.array, shape [n_validation, ]
    The values in the validation set.

reg_lambda
    : float
    The regularization strength.

max_steps
    : int, optional, default: 100
    Maximum number of training steps. Note that we will stop early if we observe
    no improvement on the validation error for a specified number of steps
    (see "patience" for details).

init
    : str in ['random', 'svd'], default 'random'
    The initialization strategy for P and Q. See function initializers for details.

log_every
    : int, optional, default: 1
    Log the training status every X iterations.

patience
    : int, optional, default: 5
    Stop training after we observe no improvement of the validation loss for
    iterations (see eval_every for details). After we stop training, we return the
    observed values for Q and P (based on the validation loss) and the best values
    for Q and P.

eval_every
    : int, optional, default: 1
    Evaluate the training and validation loss every X steps. If we observe no
    improvement on the validation loss for a specified number of steps, we stop
    training.

```

of the validation error, we decrease our patience by 1, else

Returns

best_Q : np.array, shape [N, k]
Best value for Q (based on validation loss) observed during training

best_P : np.array, shape [k, D]
Best value for P (based on validation loss) observed during training

validation_losses : list of floats
Validation loss for every evaluation iteration, can be used for plotting loss over time.

train_losses : list of floats
Training loss for every evaluation iteration, can be used for plotting loss over time.

converged_after : int
*it - patience*eval_every, where it is the iteration in which we converged, or -1 if we hit max_steps before converging.*

"""

```
Q,P = initialize_Q_P(M, k, init)
```

```
best_Q = Q
```

```
best_P = P
```

```
best_loss = -1
```

```
validation_losses = []
```

```
train_losses = []
```

```
converged_after = -1
```

```
train_idx = tuple(non_zero_idx.T)
```

```
reg = Ridge(alpha=reg_lambda, fit_intercept=False)
```

```
nnz_mask = sp.coo_matrix((np.ones(len(non_zero_idx)),  
                          (non_zero_idx[:,0],non_zero_idx[:,1])),  
                          shape=M.shape, dtype="uint8").tocsr()
```

```
rows = nnz_mask.tolil().rows
```

```
cols = nnz_mask.T.tolil().rows
```

```
for i in range(max_steps):
```

```
    if i % eval_every == 0:
```

```
        # evaluate losses
```

```
        val_loss = loss(val_values, val_idx, Q, P, reg_lambda)
```

```
        validation_losses.append(val_loss)
```

```
        train_loss = loss(M[train_idx].A1, train_idx, Q, P, reg_lambda)
```

```

train_losses.append(train_loss)

if best_loss <= -1 or val_loss < best_loss:
    best_Q = Q
    best_P = P
    best_loss = val_loss
    current_patience = patience
else:
    current_patience -= 1

if current_patience == 0:
    converged_after = i - patience * eval_every
    break

print("Iteration ", i)

# fix Q
for rating_idx in range(M.shape[1]):
    nnz_idx = cols[rating_idx]
    res = reg.fit(Q[nnz_idx], np.squeeze(M[nnz_idx, rating_idx].toarray()))
    P[:, rating_idx] = res.coef_

# fix P
for user_idx in range(M.shape[0]):
    nnz_idx = rows[user_idx]
    res = reg.fit(P[:, nnz_idx].T, np.squeeze(M[user_idx, nnz_idx].toarray()))
    Q[user_idx, :] = res.coef_

return best_Q, best_P, validation_losses, train_losses, converged_after

```

1.2.3 Train the latent factor (nothing to do here)

```

In [16]: Q, P, val_loss, train_loss, converged = latent_factor_alternating_optimization(M_shift,
                                                                                       k=100,
                                                                                       val_val=0.01,
                                                                                       reg_lambda=0.01,
                                                                                       max_steps=10000)

```

```

Iteration 0
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
Iteration 33
Iteration 34
Iteration 35
Iteration 36
Iteration 37
Iteration 38
Iteration 39
Iteration 40
Iteration 41
Iteration 42
Iteration 43
Iteration 44
Iteration 45
Iteration 46
Iteration 47
Iteration 48
Iteration 49
Iteration 50
Iteration 51
Iteration 52
Iteration 53
Iteration 54
Iteration 55
Iteration 56
Iteration 57

Iteration 58
Iteration 59
Iteration 60
Iteration 61
Iteration 62
Iteration 63
Iteration 64
Iteration 65
Iteration 66
Iteration 67
Iteration 68
Iteration 69
Iteration 70
Iteration 71
Iteration 72
Iteration 73
Iteration 74
Iteration 75
Iteration 76
Iteration 77
Iteration 78
Iteration 79
Iteration 80
Iteration 81
Iteration 82
Iteration 83
Iteration 84
Iteration 85
Iteration 86
Iteration 87
Iteration 88
Iteration 89
Iteration 90
Iteration 91
Iteration 92
Iteration 93
Iteration 94
Iteration 95
Iteration 96
Iteration 97
Iteration 98
Iteration 99

1.2.4 Plot the validation and training losses over for each iteration (nothing to do here)

```
In [17]: fig, ax = plt.subplots(1, 2, figsize=[10, 5])  
         fig.suptitle("Alternating optimization, k=100")
```

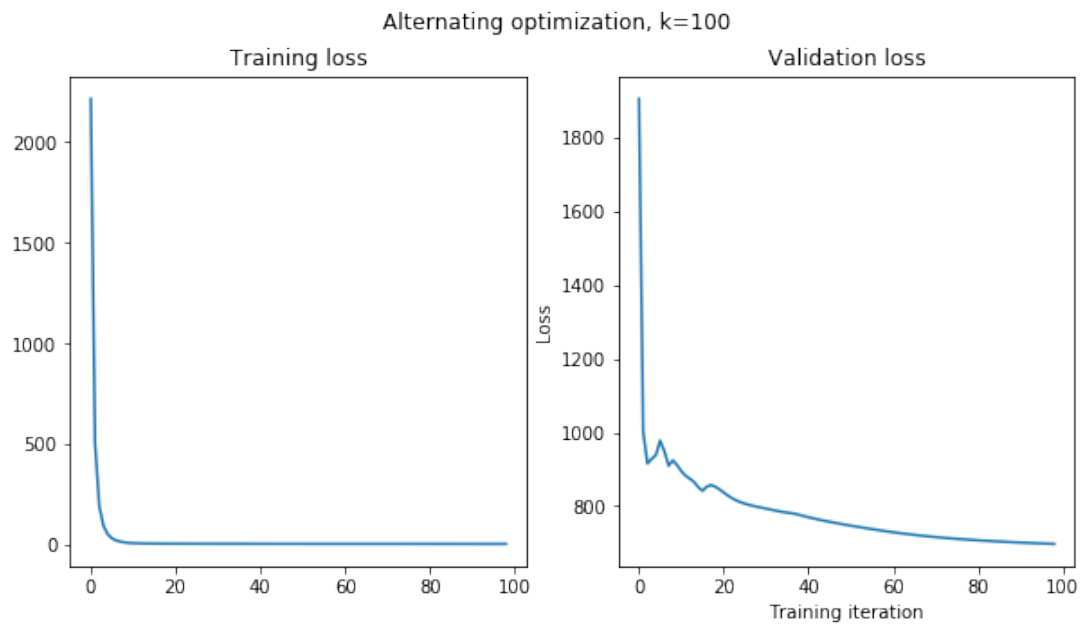
```

ax[0].plot(train_loss[1::])
ax[0].set_title('Training loss')
plt.xlabel("Training iteration")
plt.ylabel("Loss")

ax[1].plot(val_loss[1::])
ax[1].set_title('Validation loss')
plt.xlabel("Training iteration")
plt.ylabel("Loss")

plt.show()

```



In []:

Problem 2:

(Linear) Autoencoder:

Input data X : D -dimensional

Hidden layer: K -dimensional

No biases, activations = identity.

This results in a linear transformation: $f(x) = f_{dec}(f_{enc}(x)) = XW_1W_2$

With dimensions: $X : N \times D, W_1 : D \times K, W_2 : K \times D$

With $K < D$, XW_1 forces X into a K dimensional subspace.

Since this transformation is not the identity ($K < D$) perfect reconstruction is not achievable unless the input data X is already in a K -dimensional subspace despite being D -dimensional data.

Problem 3:

K Gaussians:

Intuition: Expected value of Gaussian is the mean.

\implies Expected value of K Gaussians should be the K means added up (each cluster z).

$$p(x) = \sum_k \pi_k \mathcal{N}(x | \mu_k, \Sigma_k)$$

$$\mathbb{E}[x] = \mathbb{E}_{p(z)}[\mathbb{E}_{p(x|z)}[x|z]]$$

$\mathbb{E}_{p(x|z)}[x|z]$ is the expected value of x in cluster z which is the mean of cluster z .

This implies $\mathbb{E}_{p(x|z)}[x|z] = \mu_k$.

$\mathbb{E}_{p(z)}$ is the prior probability π_z of z , also have to consider all clusters.

This implies $\mathbb{E}_{p(z)} = \sum_{k=1}^K \pi_k$.

Simply filling into the equation yields: $\mathbb{E}[x] = \sum_{k=1}^K \pi_k \mu_k$

Now $Cov[x]$:

$\mathbb{E}[x]$ and $\mathbb{E}[x]^T$ respectively are already known.

$$Cov[x] = \mathbb{E}[xx^T] - \mathbb{E}[x]\mathbb{E}[x]^T$$

So only $\mathbb{E}[xx^T]$ is still missing:

Filling into $\mathbb{E}[x] = \mathbb{E}_{p(z)}[\mathbb{E}_{p(x|z)}[x|z]]$:

$$\begin{aligned} \mathbb{E}[xx^T] &= \mathbb{E}_{p(z)}[\mathbb{E}_{p(x|z)}[xx^T|z]] \\ \mathbb{E}[xx^T] &= \sum_{k=1}^K \pi_k \mathbb{E}_{p(x|z)}[xx^T|z] \end{aligned}$$

With $\Sigma = \mathbb{E}[(X - \mu)(X - \mu)^T] = \mathbb{E}[XX^T] - \mu\mu^T$

$$\implies \mathbb{E}[XX^T] = \Sigma + \mu\mu^T$$

$$\begin{aligned} \mathbb{E}[xx^T] &= \sum_{k=1}^K \pi_k (\Sigma_k + \mu_k \mu_k^T) \\ \implies Cov[x] &= \sum_{k=1}^K \pi_k (\Sigma_k + \mu_k \mu_k^T) - \sum_{k=1}^K \sum_{l=1}^K \pi_k \pi_l \mu_k \mu_l^T \end{aligned}$$

Problem 4:

a) According to slide 12-19, we first need to draw the cluster indicators k, l from categorical distribution given the probabilities π_k^x, π_l^y

$$k \sim Cat(\pi_k^x)$$

$$l \sim Cat(\pi_l^y)$$

and then sample from their respective normal distributions:

$$x \sim \mathcal{N}(\mu_k^x, \Sigma_k^x)$$

$$y \sim \mathcal{N}(\mu_l^y, \Sigma_l^y)$$

z is then given by $z := x + y$

b) Since x and y are i.i.d and $x \sim \mathcal{N}(\mu_k^x, \Sigma_k^x)$ and $y \sim \mathcal{N}(\mu_l^y, \Sigma_l^y)$, the sum of two Gaussian distributions is again Gaussian. Therefore $p(z | \theta^x, \theta^y)$ is a mixture of Gaussians.

c)

$$p(z | \theta^x, \theta^y) = \sum_{k=1}^{K_x} \sum_{l=1}^{K_y} \pi_k^x \pi_l^y \mathcal{N}(z | \mu_k^x + \mu_l^y, \Sigma_k^x + \Sigma_l^y)$$

Problem 5:

exercise_12_clustering

February 2, 2020

0.1 Exporting the results to PDF

Once you complete the assignments, export the entire notebook as PDF and attach it to your homework solutions. The best way of doing that is 1. Run all the cells of the notebook. 2. Export/download the notebook as PDF (File -> Download as -> PDF via LaTeX (.pdf)). 3. Concatenate your solutions for other tasks with the output of Step 2. On linux, you can use `pdffunite`, there are similar tools for other platforms, too. You can only upload a single PDF file to Moodle.

Make sure you are using `nbconvert` version 5.5 or later by running `jupyter nbconvert --version`. Older versions clip lines that exceed page width, which makes your code harder to grade.

```
In [2]: import matplotlib.pyplot as plt
import numpy as np
from PIL import Image
from sklearn.datasets import load_sample_image

%matplotlib inline

def compare_images(img, img_compressed, k):
    """Show the compressed and uncompressed image side by side.
    """

    fig, axes = plt.subplots(1, 2, figsize=(16, 12))
    axes[0].set_axis_off()
    if isinstance(k, str):
        axes[0].set_title(k)
    else:
        axes[0].set_title(f"Compressed to {k} colors")
    axes[0].imshow(img_compressed)
    axes[1].set_axis_off()
    axes[1].set_title("Original")
    axes[1].imshow(img)
```

1 K-Means

In this first section you will implement the image compression algorithm from Bishop, chapter 9.1.1. Take an RGB image $X \in \mathbb{R}^{h \times w \times 3}$ and interpret it as a data matrix $X \in \mathbb{R}^{N \times 3}$. Now apply

k -means clustering to find k colors that describe the image well and replace each pixel with its associated cluster.

```
In [4]: # Alternatively try china.jpg
        X = load_sample_image("flower.jpg")

        # or load your own image
        # X = np.array(Image.open("/home/user/path/to/some.jpg"))

In [3]: def kmeans(X, k):
        """Compute a  $k$ -means clustering for the data  $X$ .

        Parameters
        -----
         $X$  : np.array of size  $N \times D$ 
            where  $N$  is the number of samples and  $D$  is the data dimensionality
         $k$  : int
            Number of clusters

        Returns
        -----
         $\mu$  : np.array of size  $k \times D$ 
            Cluster centers
         $z$  : np.array of size  $N$ 
            Cluster indicators, i.e. a number in  $0..k - 1$ , for each data point in  $X$ 
        """

        # TODO: Compute  $\mu$  and  $z$ 

        N, D = X.shape

        # 1. Initialize the centroids at random
        #  $\mu = X.\max() * \text{np.random.random}((k, D)) + X.\min()$ 
        mu = np.array([ X[np.random.randint(0, N)] for _ in range(k) ])
        z = np.zeros(N, dtype=np.int8)

        # 1. Initialize the centroids with K-means++
        mu = np.empty((k, D))
        # 1.1 Choose random centroid  $\mu_1$ 
        mu[0] = X[np.random.randint(N)]
        # 1.2 For each  $x_i$  compute Distance  $D_i^2$ 
        Di2 = np.linalg.norm(X - mu[0], axis=1) ** 2
        for i in range(1, k):
            # 1.3 Sample the next centroid  $\mu_i$  from  $\{x_i\}$  with probability proportional
            potential = Di2.sum()
            sample = np.random.random_sample(1) * potential # only 1 but could be multiple
            candidate = np.searchsorted(np.cumsum(Di2), sample)
            mu[i] = X[candidate]
```

```

        # 1.4 Recompute distance Di2
        Di2 = np.minimum(Di2, np.linalg.norm(X - mu[i], axis=1) ** 2)
    # 1.5 Continue Steps 3 and 4 und all k have been chosen

    # 2. Update cluster indicators
    for i, x in enumerate(X):
        cluster = np.argmin(np.linalg.norm(x - mu, axis=1) ** 2)
        z[i] = int(cluster)

    # 3. Update centroids
    for i in range(k):
        mask = z == i
        N_k = np.sum(mask)
        mu[i] = (1 / N_k) * np.sum(X[mask])

    # 4. Has objective converged
    if np.isnan(mu).any():
        print("Contained empty clouds")
        print(mu)
        #return kmeans(X, k)

    return mu, z

```

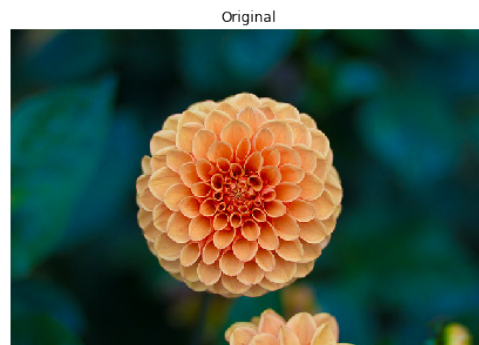
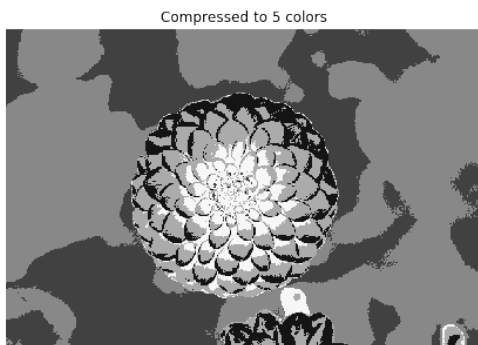
```

In [4]: # Cluster the color values
        k = 5
        mu, z = kmeans(X.reshape((-1, 3)), k)

        # Replace each pixel with its cluster color
        X_compressed = mu[z].reshape(X.shape).astype(np.uint8)

        # Show the images side by side
        compare_images(X, X_compressed, k)

```



2 Gaussian Mixture Models & EM

Now you will repeat the same exercise with GMMs.

```
In [1]: def gmm_log_probability(X, pi, mu, sigma):
    """Compute the joint log-probabilities for each data point and component.

    Parameters
    -----
    X : np.array of size N x D
        where N is the number of samples and D is the data dimensionality
    pi : np.array of size k
        Prior weight of each component
    mu : np.array of size k x D
        Mean vectors of the k Gaussian component distributions
    sigma : np.array of size k x D x D
        Covariance matrices of the k Gaussian component distributions

    Returns
    -----
    P : np.array of shape N x k
        P[i, j] is the joint log-probability of data point i under component j
    """

    # TODO: Compute P

    # log p(X, Z | , t, )
    N, D = X.shape
    k = pi.shape[0]

    #s1 = 1 / (np.sqrt( 2 * np.pi * sigma))
    #s2 = np.exp(-(np.square(X - mu) / (2 * sigma)))
    #P = pi * s1 * s2
    #print(P.shape)

    from scipy.stats import multivariate_normal
    P = np.empty((N, k))
    for i in range(k):
        P[i] = np.log(pi[i] * multivariate_normal.pdf(X, mu[i], sigma[i]))

    return P

def em(X, k, tol=0.001):
    """Fit a Gaussian mixture model with k components to X.

    Parameters
```

```

-----
X : np.array of size N x D
    where N is the number of samples and D is the data dimensionality
k : int
    Number of clusters
tol : float
    Converge when the increase in the mean of the expected joint log-likelihood
    is lower than this

The algorithm should stop when the relative improvement in the optimization
objective is less than rtol.

Returns
-----
pi : np.array of size k
    Prior weight of each component
mu : np.array of size k x D
    Mean vectors of the k Gaussian component distributions
sigma : np.array of size k x D x D
    Covariance matrices of the k Gaussian component distributions
"""

# https://github.com/scikit-learn/scikit-learn/blob/a95203b/sklearn/mixture/gmm.py

# TODO: Compute pi, mu, sigma
N, D = X.shape

# 1. Initialize model parameters
pi = np.ones(k)
mu = np.random.random((k, D))
sigma = np.array([np.identity(D) for i in range(k)])

from scipy.stats import multivariate_normal

num_iters = 0
converged = False
#while not(converged):
while num_iters < 5:
    # 2. E step. Evaluate the responsibilities
    gamma = np.zeros((N, k), dtype=float)
    for i in range(k):
        gamma[:,i] = pi[i] * multivariate_normal.pdf(X, mu[i,:], sigma[i])
    gamma_norm = np.sum(gamma, axis=1)[:,np.newaxis]
    gamma /= gamma_norm

    # 3. M step. Re-estimate the parameters
    pi = np.mean(gamma, axis=0)
    mu = np.dot(gamma.T, X) / np.sum(gamma, axis=0)[:,np.newaxis]

```

```

for i in range(k):
    x = X - mu[i,:]
    x_mu = np.matrix(x)
    gamma_diag = np.diag(gamma[:,i])
    gamma_diag = np.matrix(gamma_diag)
    sigma_i = x.T * gamma_diag * x
    sigma[i,:,:] = (sigma_i) / np.sum(gamma, axis=0)[:,np.newaxis]
    #sigma[i] = (1 / N_k) * np.sum(gamma[i] * np.square(X - mu[i]).T)

print(gamma)
print(mu)
print(sigma)
print(pi)
#likelihood = gmm_log_probability(X, pi, mu, sigma)
#if likelihood <= tol:
#    converged = True

print(likelihoods.shape)
print(np.mean(likelihoods))
# test
converged = True

num_iters += 1

return pi, mu, sigma

```

```

In [ ]: # Fit the GMM
k = 5
pi, mu, sigma = em(X.reshape((-1, 3)), k)

# Determine the most likely cluster of each pixel
log_p = gmm_log_probability(X.reshape((-1, 3)), pi, mu, sigma)
z = log_p.argmax(axis=1)

# Replace each pixel with its cluster mean
X_compressed = mu[z].reshape(X.shape).astype(np.uint8)

# Show the images side by side
compare_images(X, X_compressed, k)

```

/Users/lilith/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:88: RuntimeWarning:

3 Sampling Unseen Datapoints

You have trained a generative model which allows you to sample from the learned distribution. In this section, you sample new images.

```

In [ ]: def gmm_sample(N, pi, mu, sigma):
        """Sample N data points from a Gaussian mixture model.

        Parameters
        -----
        N : int
            Number of data points to sample
        pi : np.array of size k
            Prior weight of each component
        mu : np.array of size k x D
            Mean vectors of the k Gaussian component distributions
        sigma : np.array of size k x D x D
            Covariance matrices of the k Gaussian component distributions

        Returns
        -----
        X : np.array of shape N x D
        """

        # TODO: Sample X

        return X

In [ ]: # Sample pixels and reshape them into the size of the original image
        X_sampled = gmm_sample(np.prod(X.shape[:-1]), pi, mu, sigma).reshape(X.shape).astype(np.float32)

        # Compare the original and the sampled image
        compare_images(X, X_sampled, "Sampled")

```

Explain what you see in the generated images. (1-3 sentences)

Appendix

We confirm that the submitted solution is original work and was written by us without further assistance.
Appropriate credit has been given where reference has been made to the work of others.

Munich, February 2, 2020, Signature Marcel Bruckner (03674122)

Munich, February 2, 2020, Signature Julian Hohenadel (03673879)

Munich, February 2, 2020, Signature Kevin Bein (03707775)