Lab 8: Matrix Factorization

NOTE: This is a lab project accompanying the following book [MLT] and it should be used together with the book.

[MLT] H. Jiang. Machine Learning Fundamentals. A Concise Introduction. Cambridge University Press, 2021. (bibtex)

The aim of this lab is to explore the application of machine learning techniques to the large-scale matrix factorization problem, which has numerous practical uses, such as collaborative filtering for recommendations and latent semantic analysis (LSA) in natural language processing. Specifically, we will employ LSA on the well-known wine80 dataset as a case study to demonstrate how machine learning methods can be used to factorize large-scale sparse matrices derived from extensive text corpora. This will include efficient computation of the loss function, optimization of the loss function using various methods such as the alternating algorithm and stochastic gradient descent (SGD), and a discussion of their practical advantages and disadvantages.

Prerequisites: basic understanding on JAX, including `jax.numpy` and `jax.grad`.

Example B.1:

(see 3/1/2021 13:00:00) to construct the word-document matrix (as in Example 7.11 on page 142) for the top 10000 most frequent words in the enwiki8 dataset, where each paragraph in a line is treated as a document. Next, use `numpy` to implement the Alternating algorithm (Algorithm 7.4 on page 140) to factorize the word-document matrix to derive word vectors with dimension $k = 20$. Furthermore, use the `%timeit` method to visualize the top-500 most-frequent words to inspect their semantic relationships. At last, compare the execution times of the alternating algorithm for various word vector dimensions $k = 10, 20, 30$.

```
# !wget http://www.cse.ust.hk/~dekai/enwiki8.zip
# !unzip enwiki8.zip

# !pip install scipy
# !pip install jax jaxlib

with open('enwiki8.txt', 'r') as f:
    lines = f.readlines()
    text = ''

    for line in lines:
        text.append(line)

print(len(text))
```

```
100000
```

```
# create word-document matrix using scikit-learn

from sklearn.feature_extraction.text import CountVectorizer

vectorizer = CountVectorizer(max_features=10000) # vocabulary size = 10000
X = vectorizer.fit_transform(text).transpose() # X: word-by-document matrix (scipy.sparse.csr_matrix)
print(X.shape) # (# words by document)
print(X.count_nonzero()) # num of non-zero elements

dict = vectorizer.get_feature_names_out() # dictionary
print(len(dict))
```

```
10000
10000
```

In this laboratory exercise, we use a variation of the loss function $Q(\mathbf{U}, \mathbf{V})$ presented on page 143. Instead of summing the terms in the loss function, we calculate their average as follows:

$$Q(\mathbf{U}, \mathbf{V}) = \frac{1}{|\Omega|} \sum_{(i,j) \in \Omega} \left(x_{ij} - \mathbf{u}_i^T \mathbf{v}_j \right)^2 + \frac{\lambda}{|\mathbb{U}|} \sum_{\mathbf{u} \in \mathbb{U}} \|\mathbf{u}\|^2 + \frac{\lambda}{|\mathbb{V}|} \sum_{\mathbf{v} \in \mathbb{V}} \|\mathbf{v}\|^2$$

where $|\Omega|$ denotes the total number of training samples, and $|\mathbb{U}|$ and $|\mathbb{V}|$ stand for the number of elements in matrices $\mathbf{U}$ and $\mathbf{V}$.

```
import numpy as np

### the loss function Q(U,V) as above
### naive implementation as loops (NOTE: this function runs VERY SLOWLY)
# U_fact: word-factor matrix of dimension m x k
# V_fact: term-factor matrix of dimension n x k
def loss_fun(X, U, V, lambda=0.0, lambda=0.0):
    m, k = U.shape
    n = V.shape[0]
    loss = 0.0
    for i in range(m):
        for j in X[i,:].nonzero()[1]:
            loss += (X[i,j] - U[i,:].dot(V[j,:]))**2
    loss += lambda*np.sum(U**2)/m + lambda*np.sum(V**2)/n
    return loss

# vectorized version of loss function Q(U,V) as above
# U_fact: word-factor matrix of dimension m x k
# V_fact: term-factor matrix of dimension n x k
def loss_fun_vec(X, U, V, lambda=0.0, lambda=0.0):
    m, k = U.shape
    diff = np.sum(X.multiply(-2*U.dot(V.T)).data**2) + np.array(X.power(2).sum()).squeeze()
    loss = np.mean(diff)+k*(
    loss += lambda*np.sum(U**2)/m + lambda*np.sum(V**2)/n
    return loss
```

```
# compare running times of these two implementations of the same loss function

k=10  # with k=10
U = 0.01*np.random.normal(size=(X.shape[0], k))
V = 0.01*np.random.normal(size=(X.shape[1], k))
print("loss function is computed by loops")
print("loss = %.2f" % loss_fun(X, U, V))
print("loss function is computed via vectorization")
%timeit -n1 -r1 loss_fun_vec(X, U, V)

U = loss_fun(X, U, V)
V = loss_fun_vec(X, U, V)
print(U.shape)

loss function is computed by loops
8421.34s ± 0 ns per loop (mean ± std. dev. of 1 run, 1 loop each)
loss function is computed via vectorization
9.41 ± 0 ns per loop (mean ± std. dev. of 1 run, 1 loop each)
5.541169787925132 5.541169787925132
(10000, 10)
```

```
### Alternating Algorithm for Matrix Factorization (Algorithm 7.6 on page 145)

# U: m x k matrix
# V: n x k matrix
# U_fact: m x k matrix (scipy.sparse.csr_matrix)
def Alternating_MF(X, k=10, lambda=0.0, lambda=0.0, max_epoch=30):
    # initialize U and V
    U = 0.01*np.random.normal(size=(X.shape[0], k))
    V = 0.01*np.random.normal(size=(X.shape[1], k))
    m = X.count_nonzero() # number of training samples

    loss = loss_fun_vec(X, U, V, lambda, lambda)
    print("epoch = 0: loss = %.2f" % loss)

    for ep in range(max_epoch):
        for j in range(X.shape[0]):
            X_row = X.getrow(j)  # extract j-th row in X
            U[j,:] = X_row.dot(V).dot(np.linalg.inv(V.T.dot(V) + lambda*np.identity(k))) # U_j = X_j*V*inv(V.T*V)

        for j in range(X.shape[1]):
            X_col = X.getcol(j).transpose() # extract j-th col in X
            V[j,:] = X_col.dot(U).dot(np.linalg.inv(U.T.dot(U) + lambda*np.identity(k))) # V_j = X_j*U*inv(U.T*U)

        loss = loss_fun_vec(X, U, V, lambda, lambda)
        print("epoch = %d: loss = %.2f" % (ep+1, loss))

    return U, V
```

```
print(X.shape)

U, V = Alternating_MF(X, k=20)
```

```
(10000, 40000)
epoch = 0: loss = 5.56
epoch = 1: loss = 0.58
epoch = 2: loss = 0.41
epoch = 3: loss = 0.34
epoch = 4: loss = 0.31
epoch = 5: loss = 0.29
epoch = 6: loss = 0.28
epoch = 7: loss = 0.27
epoch = 8: loss = 0.26
epoch = 9: loss = 0.26
epoch = 10: loss = 0.25
epoch = 11: loss = 0.25
epoch = 12: loss = 0.25
epoch = 13: loss = 0.25
epoch = 14: loss = 0.25
epoch = 15: loss = 0.25
epoch = 16: loss = 0.25
epoch = 17: loss = 0.25
epoch = 18: loss = 0.25
epoch = 19: loss = 0.25
epoch = 20: loss = 0.25
(10000, 20)
```

```
# train SVDs to project word vectors to 2-d space for visualization

from sklearn.manifold import TSNE

print(U.shape, V.shape)

tsne_model_2d = TSNE(perplexity=15, n_components=2, init='pca', n_iter=3500, random_state=12)
U_2d = tsne_model_2d.fit_transform(U)

print(U_2d.shape)
```

```
(10000, 20) (40000, 20)
(10000, 2)
```

```
# use matplotlib to display term representation words using their SVD2 projections in a 2-D plane

import matplotlib.pyplot as plt
import matplotlib.cm as cm

words = ["the","about","would","what","how","can","create","disaster","scientific","family","film","food","history",
         "hospital","hotel","love","movie","money","moon","music","peace","shape","woman","world","travel","tiger",
         "ancient","cow","secretary","professor","river","president","prefix","price","nurse","war","marriage","example",
         "four","fruit","japanese","planet","sing","queen","water","science","reason"]

x = []
y = []
idx = []

indices = np.random.permutation(len(some_words))

for wd in some_words[:indices]:
    if (wd.where(dict == wd)[0]
        try:
            x.append(U_2d[i][0])
            y.append(U_2d[i][1])
            idx.append(i)
        except:
            pass

colors = cm.rainbow(np.linspace(0, 1, len(idx)))

for xi, yi, ci, wd in zip(x, y, colors, words):
    plt.scatter(xi, yi, color=ci)

for i, txt in enumerate(words):
    ax.annotate(txt, (x[i], y[i]))
```

```
<ipython-input-49-fb31b98f58c1>:15: DeprecationWarning: The truth value of an empty array is ambiguous. Returning False, but in future this will result in an error. Use `array.size > 0` to check that an array is not empty.
  if (wd.where(dict == wd)[0]
```

```
# compare running times of the alternative algorithm (only one epoch) for k=10,20

print('k=10')
%timeit -n1 -r1 Alternating_MF(X,k=10,max_epoch=1)

print('k=20')
%timeit -n1 -r1 Alternating_MF(X,k=20,max_epoch=1)
```

```
k=10
epoch = 0: loss = 5.56
epoch = 1: loss = 0.58
1min 21s ± 0 ns per loop (mean ± std. dev. of 1 run, 1 loop each)
k=20
epoch = 0: loss = 5.56
epoch = 1: loss = 0.58
2min 41s ± 0 ns per loop (mean ± std. dev. of 1 run, 1 loop each)
```

Example B.2:

Implement the mini-batch stochastic gradient descent (SGD) method using JAX to factorize the given word-document matrix for $k = 10, 20, 30$. Utilize JAX's automatic differentiation method `jax.grad` to compute the gradient for the specified objective function. Compare the performance of the SGD method with the previously discussed alternating algorithm in terms of execution speed.

```
### Stochastic Gradient Descent for Matrix Factorization
# use jax.grad() to compute the gradient automatically

import numpy as np
import jax.numpy as jnp
import jax.numpy as jax
from jax import grad, random, device_put

# JAX implementation of vectorized version of loss function Q(U,V) on page 143
# U_fact: word-factor matrix of dimension m x k
# V_fact: term-factor matrix of dimension n x k
def loss_fun_vec_jax(X, U, V, lambda=0.0, lambda=0.0):
    m, k = U.shape
    diff = jnp.sum(X.multiply(-2*U.dot(V.T)).data**2) + jnp.array(X.power(2).sum()).squeeze()
    loss = jnp.mean(diff)+k*(
    loss += lambda*jnp.sum(U**2)/m + lambda*jnp.sum(V**2)/n
    return loss

# U: m x k matrix (scipy.sparse.csr_matrix)
# V: n x k matrix (scipy.sparse.csr_matrix)
def SGD_MF_autograd(X, k=10, batch_size=100, lambda=0.1, lambda=0.1, max_epoch=10, lr=0.01):
    # initialize U and V
    U = device_put(0.01*random.normal(key, (X.shape[0], k)))
    V = device_put(0.01*random.normal(key, (X.shape[1], k)))
    n_index = X.nonzero()

    loss = loss_fun_vec_jax(X, U, V, lambda, lambda)
    print("epoch = 0: loss = %.2f" % loss)

    for ep in range(max_epoch):
        # X_shuffle = shuffle(X, random_state=0)  #randomly shuffle data indices
        for batch_start in range(0, X.nonzero()[0].size, batch_size):
            batch_indices = indices[batch_start:batch_start+batch_size]
            X_data = jnp.asarray(X.data[batch_indices])
            X_batch = sparse.csr_matrix((X_data,(X.nonzero()[0][batch_indices],X.nonzero()[1][batch_indices])),shape=X.shape)

            U_grad, V_grad = grad(loss_fun_vec_jax, argnums=(0,1))(U,V,X_batch)
            U = U - lr*U_grad
            V = V - lr*V_grad

        loss = loss_fun_vec(X, U, V, lambda, lambda)
        print("epoch = %d: loss = %.2f" % (ep+1, loss))

    return U, V
```

```
U, V = SGD_MF_autograd(X,k=10,batch_size=1000,lr=0.1, max_epoch=5)
```

```
epoch = 0: loss = 5.56
epoch = 1: loss = 1.56
epoch = 2: loss = 1.56
epoch = 3: loss = 1.56
epoch = 4: loss = 1.56
epoch = 5: loss = 1.56
```

```
# compare running times of different versions of loss functions

print('compute the loss function with numpy:')
%timeit loss_fun_vec(X, U, V)
print('compute the loss function with jax.numpy:')
%timeit loss_fun_vec_jax(X, U, V)

U = loss_fun_vec(X, U, V)
V = loss_fun_vec_jax(X, U, V)
print(U.T)
```

```
compute the loss function with numpy:
8.21 s ± 682 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
compute the loss function with jax.numpy:
5.03 s ± 308 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
[[ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -0.00000000e+00
  -0.00000000e+00 -0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -0.00000000e+00
  -0.00000000e+00 -0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -0.00000000e+00
  -0.00000000e+00 -0.00000000e+00]
 ...
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -0.00000000e+00
  -0.00000000e+00 -0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -0.00000000e+00
  -0.00000000e+00 -0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -0.00000000e+00
  -0.00000000e+00 -0.00000000e+00]]
```

Example B.3:

Rather than employing JAX's automatic differentiation, implement the mini-batch stochastic gradient descent (SGD) method from scratch. Specifically, manually compute the gradient for the given loss function and use it to perform SGD for matrix factorization of the word-document matrix with $k = 10$. Compare the performance of this manually implemented SGD method with the one using JAX's automatic differentiation in Example B.2 as well as the alternating algorithm in Example B.1.

Here, we first derive the formula to compute the gradient for the loss function of the form we discussed in class:

$$Q(\mathbf{U}, \mathbf{V}) = \frac{1}{|\Omega|} \sum_{(i,j) \in \Omega} \left(x_{ij} - \mathbf{u}_i^T \mathbf{v}_j \right)^2 + \frac{\lambda}{|\mathbb{U}|} \sum_{\mathbf{u} \in \mathbb{U}} \|\mathbf{u}\|^2 + \frac{\lambda}{|\mathbb{V}|} \sum_{\mathbf{v} \in \mathbb{V}} \|\mathbf{v}\|^2$$

Given any mini-batch $\mathcal{B}$ that contain indices (i, j) of some non-zero elements in $\mathbf{X}$, the objective function is written as

$$Q(\mathbf{U}, \mathbf{V}) = \frac{1}{|\mathcal{B}|} \sum_{(i,j) \in \mathcal{B}} \left(x_{ij} - \mathbf{u}_i^T \mathbf{v}_j \right)^2 + \frac{\lambda}{|\mathbb{U}|} \sum_{\mathbf{u} \in \mathbb{U}} \|\mathbf{u}\|^2 + \frac{\lambda}{|\mathbb{V}|} \sum_{\mathbf{v} \in \mathbb{V}} \|\mathbf{v}\|^2$$

where $|\mathcal{B}|$ denotes the mini-batch size, and $|\mathbb{U}|$ and $|\mathbb{V}|$ stand for the number of elements in matrices $\mathbf{U}$ and $\mathbf{V}$.

For all i in $\mathcal{B}$,

$$\frac{\partial Q}{\partial \mathbf{u}_i} = \frac{1}{|\mathcal{B}|} \sum_{(i,j) \in \mathcal{B}} 2(x_{ij} - \mathbf{u}_i^T \mathbf{v}_j)(-\mathbf{v}_j) + \frac{2\lambda}{|\mathbb{U}|} \mathbf{u}_i$$

For all j in $\mathcal{B}$,

$$\frac{\partial Q}{\partial \mathbf{v}_j} = \frac{1}{|\mathcal{B}|} \sum_{(i,j) \in \mathcal{B}} 2(x_{ij} - \mathbf{u}_i^T \mathbf{v}_j)(-\mathbf{u}_i) + \frac{2\lambda}{|\mathbb{V}|} \mathbf{v}_j$$

```
# use numpy to implement the code to compute the gradient from scratch as above
import numpy as np

def my_grad(X, U, V, batch, lambda=0.1, lambda=0.1):
    m, k = U.shape
    U_grad = np.zeros_like(U)
    n = X.batch_nonzero()
    n = X.batch_count_nonzero()

    diff = np.sum(X[batch,:].multiply(-2*U[batch,:].dot(V.T)).data**2) + np.array(X[batch,:].power(2).sum()).squeeze()
    for i in batch:
        U_grad[i,:] = (2 / n) * (-V).dot(X[i,:].todense().T) + (2 * lambda/m)*U[i,:]
        V_grad[i,:] = (2 / n) * (-U).dot(X[i,:].todense()) + (2 * lambda/n)*V[i,:]

    return U_grad, V_grad
```

```
# U: m x k matrix (scipy.sparse.csr_matrix)
# V: n x k matrix (scipy.sparse.csr_matrix)
def SGD_MF(X, k=10, batch_size=100, lambda=0.1, lambda=0.1, max_epoch=10, lr=0.01):
    # initialize U and V
    U = 0.01*np.random.normal(size=(X.shape[0], k))
    V = 0.01*np.random.normal(size=(X.shape[1], k))
    n_index = X.nonzero()

    loss = loss_fun_vec(X, U, V, lambda, lambda)
    print("epoch = 0: loss = %.2f" % loss)

    for ep in range(max_epoch):
        # X_shuffle = shuffle(X, random_state=0)  #randomly shuffle data indices
        for batch_start in range(0, X.nonzero()[0].size, batch_size):
            batch_indices = indices[batch_start:batch_start+batch_size]
            X_data = np.asarray(X.data[batch_indices])
            X_batch = sparse.csr_matrix((X_data,(X.nonzero()[0][batch_indices],X.nonzero()[1][batch_indices])),shape=X.shape)

            U_grad, V_grad = my_grad(U, V, X_batch)
            U = U - lr*U_grad
            V = V - lr*V_grad

        loss = loss_fun_vec(X, U, V, lambda, lambda)
        print("epoch = %d: loss = %.2f" % (ep+1, loss))

    return U, V
```

```
print("SGD with my_grad() with batch_size = 1000:")
%timeit -n1 -r1 SGD_MF(X,k=10,batch_size=1000,lr=0.1,max_epoch=1)

print("SGD with my_grad() with batch_size = 100:")
%timeit -n1 -r1 SGD_MF(X,k=10,batch_size=100,lr=0.1,max_epoch=1)
```

```
SGD with my_grad() with batch_size = 1000:
epoch = 0: loss = 5.56
epoch = 1: loss = 0.59
1min 53s ± 0 ns per loop (mean ± std. dev. of 1 run, 1 loop each)
SGD with my_grad() with batch_size = 100:
epoch = 0: loss = 5.56
epoch = 1: loss = 0.58
2min 27s ± 0 ns per loop (mean ± std. dev. of 1 run, 1 loop each)
```

```
print("SGD with my_grad() with batch_size = 500:")
%timeit -n1 -r1 SGD_MF(X,k=10,batch_size=500,lr=0.1,max_epoch=1)
```

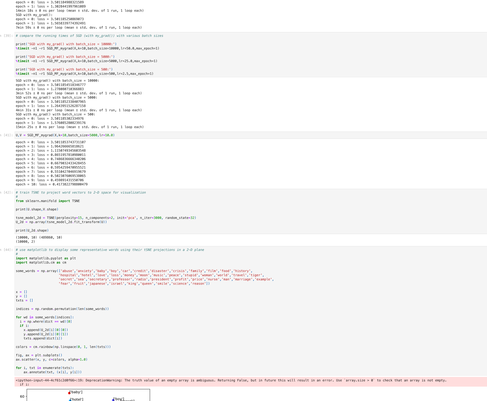
```
SGD with my_grad() with batch_size = 500:
epoch = 0: loss = 5.56
epoch = 1: loss = 0.58
1min 59s ± 0 ns per loop (mean ± std. dev. of 1 run, 1 loop each)
```

```
# train SVDs to project word vectors to 2-d space for visualization

from sklearn.manifold import TSNE

tsne_model_2d = TSNE(perplexity=15, n_components=2, init='pca', n_iter=3500, random_state=12)
U_2d = tsne_model_2d.fit_transform(U)

print(U_2d.shape)
```

```
(10000, 2)
```

```
# use matplotlib to display some representative words using their SVD2 projections in a 2-D plane

import matplotlib.pyplot as plt
import matplotlib.cm as cm

words = ["the","about","would","what","how","can","create","disaster","scientific","family","film","food","history",
         "hospital","hotel","love","movie","money","moon","music","peace","shape","woman","world","travel","tiger",
         "ancient","cow","secretary","professor","river","president","prefix","price","nurse","war","marriage","example",
         "four","fruit","japanese","planet","sing","queen","water","science","reason"]

x = []
y = []
idx = []

indices = np.random.permutation(len(some_words))

for wd in some_words[:indices]:
    if (wd.where(dict == wd)[0]
        try:
            x.append(U_2d[i][0])
            y.append(U_2d[i][1])
            idx.append(i)
        except:
            pass

colors = cm.rainbow(np.linspace(0, 1, len(idx)))

for xi, yi, ci, wd in zip(x, y, colors, words):
    plt.scatter(xi, yi, color=ci)

for i, txt in enumerate(words):
    ax.annotate(txt, (x[i], y[i]))
```

```
<ipython-input-48-fb31b98f58c1>:15: DeprecationWarning: The truth value of an empty array is ambiguous. Returning False, but in future this will result in an error. Use `array.size > 0` to check that an array is not empty.
  if (wd.where(dict == wd)[0]
```



Exercises

Problem B.1:

To assess the quality of word vectors, we can compare the similarities between the derived word vectors to the semantic similarities annotated by humans for the same words. The `WordSim353` dataset provides human-assigned similarity scores for approximately 353 word pairs. For each pair of words in `WordSim353`, calculate the cosine distance between the corresponding derived word vectors. Then, compute the Pearson correlation coefficient between these cosine distances and the human-assigned scores. Discuss the findings from this analysis.

```
# Download WordSim353 dataset from Google Drive
# !gdown https://drive.google.com/file/d/1rGxfORiMnzC4vOpgyYj2ue4mKTHLK3bN/ -O data/ws353.zip

# In download WordSim353 dataset from forhd server
# !wget http://www.cse.ust.hk/~dekai/wang/wordsim353_human_scores.txt
```

Problem B.2:

Use either the alternating algorithm or gradient descent method to implement collaborative filtering for a movie recommendation task on the Netflix Prize dataset.