Homework 5-6

November 3, 2023

1 Lab: SVD and PCA

1.1 1 SVD and PCA basics

Create test data array A.

[ ]:
```
import numpy as np

a = np.array([
    [17, 24, 1, 8, 15],
    [23, 5, 7, 14, 16],
    [4, 6, 13, 20, 22],
    [10, 12, 19, 21, 3],
    [11, 18, 25, 2, 9]
], dtype=float)
```

1.1.1 Exercise 1

Perform singular value decomposition on A and compute fraction of explained variance for each direction in the SVD.

[ ]:
```
x, s, y = np.linalg.svd(a)

explained_var = s ** 2 / np.sum(s ** 2)
print(f'Explained variance fractions = {explained_var}')
```

```
Explained variance fractions = [0.76470588 0.09201289 0.08513021 0.03251685
0.02563417]
```

According to the NumPy documentation, `np.linalg.svd` returns the Hermitian transpose of V, which is the transpose for real matrices. We can see that treating `y` as V^T gives the correct reconstruction of A, and treating `y` as V does not.

[ ]:
```
sigma = np.zeros_like(a)
np.fill_diagonal(sigma, s)

print('Correct reconstruction (by assuming y = V^T)')
print(x @ sigma @ y)
print()
```

```
print('Incorrect reconstruction (by assuming y = V)')
print(x @ sigma @ y.T)
```

```
Correct reconstruction (by assuming y = V^T)
[[17. 24.  1.  8. 15.]
 [23.  5.  7. 14. 16.]
 [ 4.  6. 13. 20. 22.]
 [10. 12. 19. 21.  3.]
 [11. 18. 25.  2.  9.]]

Incorrect reconstruction (by assuming y = V)
[[ 27.02966724   4.90590117  12.26473669 -13.33001648  -8.49800667]
 [  9.66848684  12.62672641  20.03405011 -19.37677298  -5.02629561]
 [ 10.65697075  23.05568464   1.54933231 -21.35487499  -1.19718998]
 [  6.40628198  17.76727989   3.39085242 -15.77067109 -20.93015455]
 [ 11.23859319   0.43861409  -1.40214006 -26.49118967 -18.02089103]]
```

Assuming $y = V^T$, compute norm difference between A and the reconstruction.

[ ]:
```
b = x @ sigma @ y
print(f'All components close? {np.allclose(b, a)}')
print(f'Frobenius norm of difference = {np.linalg.norm(a - b)}')
```

```
All components close? True
Frobenius norm of difference = 8.523187293941492e-14
```

Project A to the first two principal components.

[ ]:
```
w = y.T[:, :2]
ar = a @ w
print(ar)
```

```
[[-2.90688837e+01 -1.23024779e+01]
 [-2.90688837e+01 -1.01407417e+01]
 [-2.90688837e+01 -5.31241717e-13]
 [-2.90688837e+01  1.01407417e+01]
 [-2.90688837e+01  1.23024779e+01]]
```

1.1.2 Exercise 2

Perform PCA of A using `sklearn`.

[ ]:
```
from sklearn.decomposition import PCA

pca = PCA(2)
pca.fit(a)
ar2 = pca.transform(a)
print(ar2)
```

```
[[ 1.23024779e+01 -1.10967458e+01]
 [ 1.01407417e+01  4.23857973e+00]
```

```
 [-6.25055563e-14  1.37163321e+01]
 [-1.01407417e+01  4.23857973e+00]
 [-1.23024779e+01 -1.10967458e+01]]
```

Get fraction of variance explained by each component:

[ ]:
```python
print(pca.explained_variance_ratio_)
```

```
[0.39105478 0.3618034 ]
```

The reduced matrix is not the same as what we got in Exercise 1 – `PCA` *centers* the data before performing the SVD.

[ ]:
```python
pca_full = PCA(5).fit(a)
print(np.cumsum(pca_full.explained_variance_ratio_))
```

```
[0.39105478 0.75285817 0.89105478 1.         1.        ]
```

Looking at the cumulative sum of the explained variance ratios, we see that 3 components are necessary to explain at least 80% of the variance.

1.1.3 Exercise 3

Center the data.

[ ]:
```python
a_center = a - np.mean(a, axis=1, keepdims=True)
```

Now do the SVD analysis as we did in Exercise 1.

[ ]:
```python
x, s, y = np.linalg.svd(a_center)
sigma = np.zeros_like(a)
np.fill_diagonal(sigma, s)

w = y.T[:, :2]
ar3 = a @ w
print(ar3)
```

```
[[-1.23024779e+01  1.10967458e+01]
 [-1.01407417e+01 -4.23857973e+00]
 [ 5.97299987e-14 -1.37163321e+01]
 [ 1.01407417e+01 -4.23857973e+00]
 [ 1.23024779e+01  1.10967458e+01]]
```

The reduced matrix is the same as that returned by Scikit-Learn (up to sign, which is OK because singular vectors are only defined up to a constant multiple).

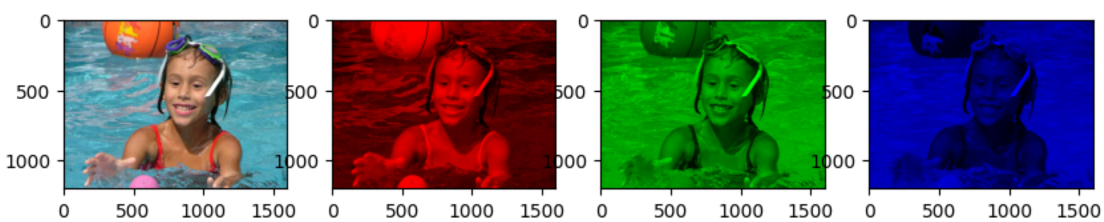
[ ]:
```python
print(f'All components close with same sign? {np.allclose(ar3, ar2)}')
print(f'All components close with opposite sign? {np.allclose(ar3, -ar2)}')
```

```
All components close with same sign? False
All components close with opposite sign? True
```

1.2 2 SVD and PCA for image compression

Load image, split into channels, and display to make sure we loaded it correctly.

[ ]:
```
import imageio
import matplotlib.pyplot as plt

image = imageio.v3.imread('swim.jpg')
red, green, blue = image.transpose((2, 0, 1))[:3]

# reproject possibly 1-channel images to RGB for display
# (RGB -> RGB, R -> RGB, G -> RGB, B -> RGB)
projections = (
    lambda im: im,
    lambda im: im[..., None] * np.array([1, 0, 0]).reshape(1, 1, 3),
    lambda im: im[..., None] * np.array([0, 1, 0]).reshape(1, 1, 3),
    lambda im: im[..., None] * np.array([0, 0, 1]).reshape(1, 1, 3),
)

_, axes = plt.subplots(1, 4, figsize=(10, 6))
for ax, channel, proj in zip(axes, (image, red, green, blue), projections):
    ax.imshow(proj(channel))
```



1.2.1 Exercise 4

Let A be one channel of our image. To compute the rank-k approximation $A^{(k)}$ of A, we use the sum

$$A^{(k)} = \sum_{j=1}^{k} \sigma_j A_j, \tag{1}$$

where $A_j = u_j \otimes v_j = u_j v_j^T$, the outer product of the left and right singular vectors u_j and v_j of A corresponding to the singular value σ_j, which is the j-th largest.

We can rewrite (1) as

$$A^{(k)} = \begin{bmatrix} u_1 & u_2 & \cdots & u_k \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_k \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_k^T \end{bmatrix}.$$

If U, d, and V^T are the matrices returned by `np.linalg.svd`, then $\{u_j\}$ are the first k columns of U, $\{v_j^T\}$ are the first k rows of V^T, and $\{\sigma_j\}$ are the first k elements of d. Therefore, equation (1) becomes

$$A^{(k)} = U_k \text{diag}_k(d) V_k^T$$

where U_k is U truncated to the first k columns, $\text{diag}_k(d)$ is the diagonal matrix with diagonal values taken from the first k values of d, and V_k^T is V^T truncated to the first k rows.

Now define a function to compute the SVD and matrix product above for $A^{(k)}$ for a given k on each channel of the image.

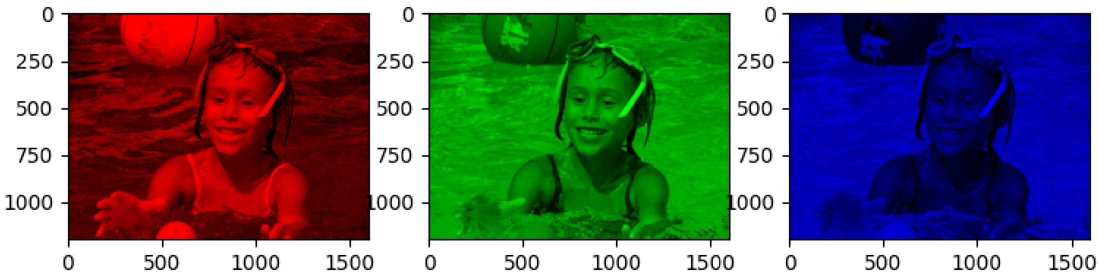
[ ]:
```
import numpy as np

def reduced_image(k):
    reduced = []
    for channel in (red, green, blue):
        # SVD (don't need to return full U and V matrices because we need k <=
 ↪rank(A) anyway)
        u, d, vt = np.linalg.svd(channel.astype(float), full_matrices=False)
        # compute rank-k approximation
        reduced.append(u[:, :k] @ np.diag(d[:k]) @ vt[:k])

    # stack reconstructed channels, clip to [0, 255], and convert back to 8-bit
 ↪unsigned integer
    return np.clip(np.stack(reduced, axis=-1), 0, 255).astype(np.uint8)
```

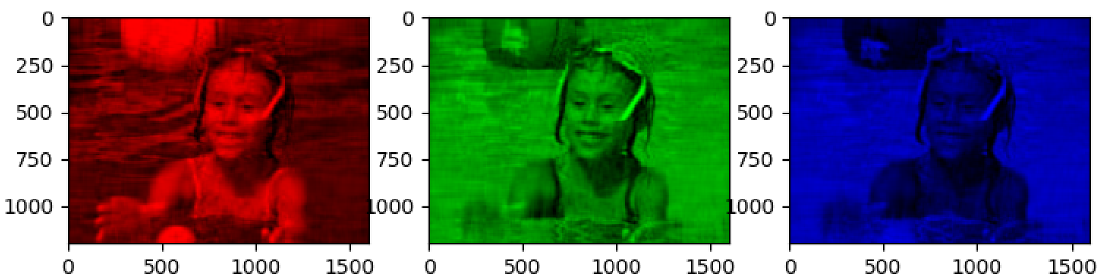
Compute the rank-20 approximation of the image.

[ ]:
```
reduced_image_20 = reduced_image(20)
```

Display original image channels and rank-20 approximations.

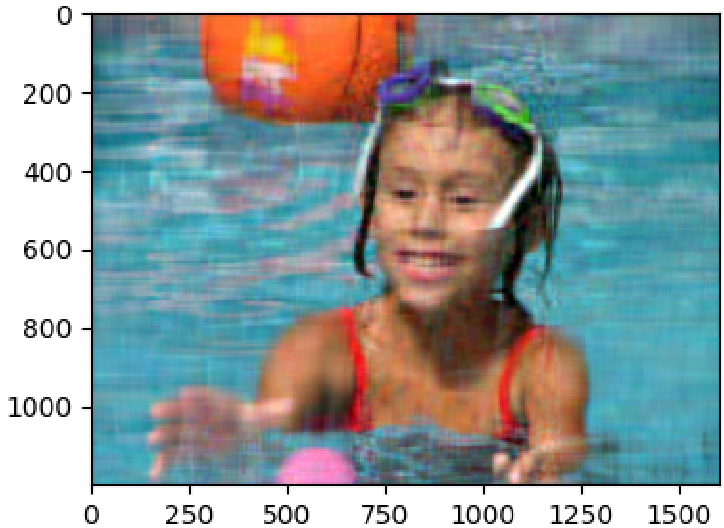
[ ]:
```
_, axes = plt.subplots(2, 3, figsize=(9, 7))
for row_axes, row_image in zip(axes, (image, reduced_image_20)):
    for ax, channel, proj in zip(row_axes, row_image.transpose((2, 0, 1)),
 ↪projections[1:]):
        ax.imshow(proj(channel))
plt.show()
```





Display original image and channel-wise rank-20 approximation.

[ ]:
```
_, axes = plt.subplots(2, 1, figsize=(6, 7))
for ax, im in zip(axes, (image, reduced_image_20)):
    ax.imshow(im)
```



1.2.2 Exercise 5

Define a function that uses PCA to compute the channel-wise rank-k approximation of the image.

[ ]:
```
from sklearn.decomposition import PCA

def reduced_image_pca(k):
    reduced = []
    for channel in (red, green, blue):
        # do PCA on the channel to get reduced representation
        pca = PCA(k)
        low_dim = pca.fit_transform(channel.astype(float))
```

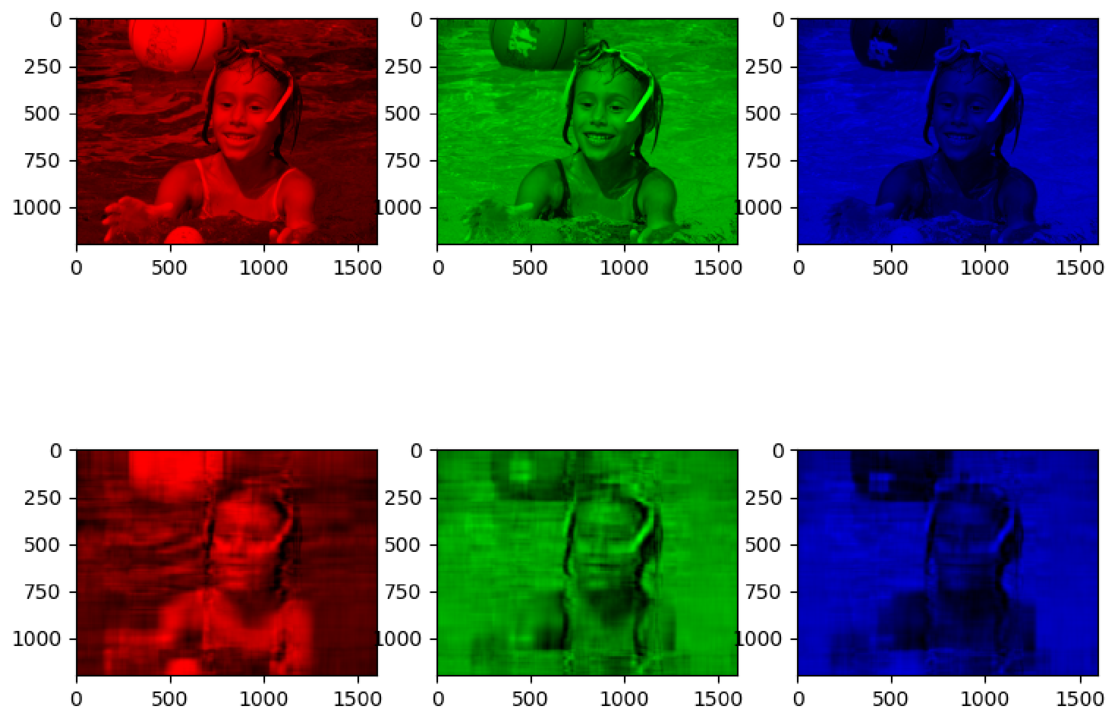
```
        # get reconstruction from reduced representation
        reduced.append(pca.inverse_transform(low_dim))

    # stack channels, clip to [0, 255], and convert back to unsigned 8-bit␣
 ↪integer
    return np.clip(np.stack(reduced, axis=-1), 0, 255).astype(np.uint8)
```

Use PCA to get rank-10 approximation of the image.

[ ]:
```
reduced_image_pca_10 = reduced_image_pca(10)
```

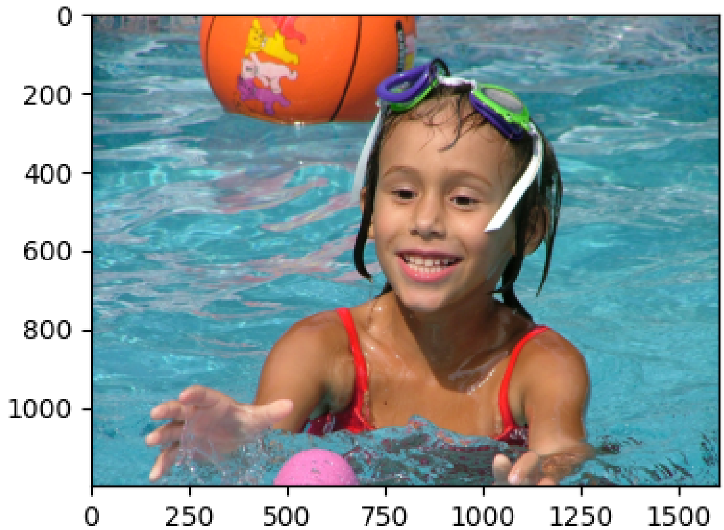
Display original image channels and rank-10 PCA approximations of each channel.

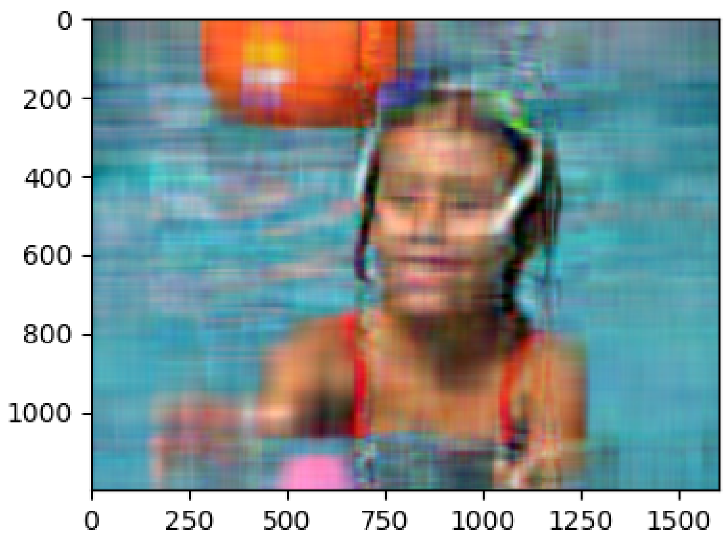
[ ]:
```
_, axes = plt.subplots(2, 3, figsize=(9, 7))
for row_axes, row_image in zip(axes, (image, reduced_image_pca_10)):
    for ax, channel, proj in zip(row_axes, row_image.transpose((2, 0, 1)),␣
 ↪projections[1:]):
        ax.imshow(proj(channel))
plt.show()
```



Display original image and rank-10 channel-wise PCA approximation.

[ ]:
```
_, axes = plt.subplots(2, 1, figsize=(6, 7))
for ax, im in zip(axes, (image, reduced_image_pca_10)):
    ax.imshow(im)
```





1.3 3 PCA for dimensionality reduction

1.3.1 Exercise 6

Load data.

[ ]:
```
import pandas
df = pandas.read_csv('diagnosis.csv')
df.head(5)
```

[ ]:
```
         id diagnosis  radius_mean  texture_mean  perimeter_mean  area_mean  \
0    842302         M        17.99         10.38          122.80     1001.0
1    842517         M        20.57         17.77          132.90     1326.0
```

```
2  84300903         M        19.69        21.25          130.00     1203.0
3  84348301         M        11.42        20.38           77.58      386.1
4  84358402         M        20.29        14.34          135.10     1297.0

   smoothness_mean  compactness_mean  concavity_mean  concave points_mean  \
0          0.11840           0.27760          0.3001              0.14710
1          0.08474           0.07864          0.0869              0.07017
2          0.10960           0.15990          0.1974              0.12790
3          0.14250           0.28390          0.2414              0.10520
4          0.10030           0.13280          0.1980              0.10430

   …  texture_worst  perimeter_worst  area_worst  smoothness_worst  \
0  …          17.33           184.60      2019.0            0.1622
1  …          23.41           158.80      1956.0            0.1238
2  …          25.53           152.50      1709.0            0.1444
3  …          26.50            98.87       567.7            0.2098
4  …          16.67           152.20      1575.0            0.1374

   compactness_worst  concavity_worst  concave points_worst  symmetry_worst  \
0             0.6656           0.7119                0.2654          0.4601
1             0.1866           0.2416                0.1860          0.2750
2             0.4245           0.4504                0.2430          0.3613
3             0.8663           0.6869                0.2575          0.6638
4             0.2050           0.4000                0.1625          0.2364

   fractal_dimension_worst  Unnamed: 32
0                  0.11890          NaN
1                  0.08902          NaN
2                  0.08758          NaN
3                  0.17300          NaN
4                  0.07678          NaN

[5 rows x 33 columns]
```

Since we are going to use the reduced data for classification, we should exclude the **diagnosis** feature from the PCA dimension reduction. We also need to exclude the erroneously loaded **Unnamed: 32** feature, and the useless **id** feature.

[ ]:
```
diagnosis = np.array([1. if d == 'M' else 0. for d in df['diagnosis']])
df = df.drop('diagnosis', axis=1)
df = df.drop('Unnamed: 32', axis=1)
df = df.drop('id', axis=1)
df.head(5)
```

[ ]:
```
   radius_mean  texture_mean  perimeter_mean  area_mean  smoothness_mean  \
0        17.99         10.38          122.80     1001.0          0.11840
1        20.57         17.77          132.90     1326.0          0.08474
2        19.69         21.25          130.00     1203.0          0.10960
```

```
3       11.42         20.38           77.58      386.1          0.14250
4       20.29         14.34          135.10     1297.0          0.10030

   compactness_mean  concavity_mean  concave points_mean  symmetry_mean  \
0           0.27760          0.3001              0.14710         0.2419
1           0.07864          0.0869              0.07017         0.1812
2           0.15990          0.1974              0.12790         0.2069
3           0.28390          0.2414              0.10520         0.2597
4           0.13280          0.1980              0.10430         0.1809

   fractal_dimension_mean  …  radius_worst  texture_worst  perimeter_worst  \
0                 0.07871  …         25.38          17.33           184.60
1                 0.05667  …         24.99          23.41           158.80
2                 0.05999  …         23.57          25.53           152.50
3                 0.09744  …         14.91          26.50            98.87
4                 0.05883  …         22.54          16.67           152.20

   area_worst  smoothness_worst  compactness_worst  concavity_worst  \
0      2019.0            0.1622             0.6656           0.7119
1      1956.0            0.1238             0.1866           0.2416
2      1709.0            0.1444             0.4245           0.4504
3       567.7            0.2098             0.8663           0.6869
4      1575.0            0.1374             0.2050           0.4000

   concave points_worst  symmetry_worst  fractal_dimension_worst
0                0.2654          0.4601                  0.11890
1                0.1860          0.2750                  0.08902
2                0.2430          0.3613                  0.08758
3                0.2575          0.6638                  0.17300
4                0.1625          0.2364                  0.07678

[5 rows x 30 columns]
```

Use PCA to reduce the dimensionality of the input features.

[ ]:
```
diagnosis_pca = PCA(2).fit(df)
dfr = diagnosis_pca.transform(df)
```

Create training and testing splits from the **reduced** data.

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

x_train, x_test, y_train, y_test = train_test_split(dfr, diagnosis, test_size=.
↪25, random_state=20)
```

Fit a logistic regression model to the training data.

[ ]:
```python
from sklearn.linear_model import LogisticRegression

model = LogisticRegression().fit(x_train, y_train)
```

Compute confusion matrices of the model on training and testing data.

[ ]:
```python
from sklearn.metrics import confusion_matrix

for x, y, name in [(x_train, y_train, 'train'), (x_test, y_test, 'test')]:
    y_pred = model.predict(x)
    print(f'Confusion matrix for {name}')
    print(confusion_matrix(y, y_pred))
    print()
```

```
Confusion matrix for train
[[261  10]
 [ 20 135]]

Confusion matrix for test
[[84  2]
 [ 7 50]]
```

1.3.2 Exercise 7

Normalize reduced data computed in the previous exercise.

[ ]:
```python
from sklearn.preprocessing import MinMaxScaler

dfr_norm = MinMaxScaler().fit_transform(dfr)
```

Now split the normalized data.

[ ]:
```python
from sklearn.model_selection import train_test_split

x_train_n, x_test_n, y_train_n, y_test_n = train_test_split(dfr_norm,␣
 ↪diagnosis, test_size=.25, random_state=20)
```

Fit a logistic regression to the normalized, reduced data.

[ ]:
```python
from sklearn.linear_model import LogisticRegression

model_n = LogisticRegression().fit(x_train_n, y_train_n)
```

Compute confusion matrices for the training and testing data.

[ ]:
```python
from sklearn.metrics import confusion_matrix

for x, y, name in [(x_train_n, y_train_n, 'train'), (x_test_n, y_test_n,␣
 ↪'test')]:
```

```python
    y_pred = model_n.predict(x)
    print(f'Confusion matrix for {name}')
    print(confusion_matrix(y, y_pred))
    print()
```

```
Confusion matrix for train
[[270   1]
 [ 60  95]]

Confusion matrix for test
[[86  0]
 [20 37]]
```