Week 5-2: Principal component analysis

Last time

- Loss function
- K-means
- GMM

Today

- GMM (cont'd)
- PCA, probabilistic PCA, functional PCA, sparse PCA, factor analysis

Reference

- Ch 14.5 of ESL
- HDS: Ch8 of Wainwright, M. J. (2019). High-dimensional Statistics. *Cambridge Series in Statistical and Probabilistic Mathematics*
- Baik, J and J. Silverman (2004). Eigenvalues of Large Sample Covariance Matrices of Spiked Population Models. *Journal of Multivariate Analysis* 97:1382--1408
- Y. Guan and J. Dy (2009). Sparse Probabilistic Principal Component Analysis. *Proceedings of the Twelth International Conference on Artificial Intelligence and Statistics*, PMLR 5:185-192
- D. Paul (2007). Asymptotics of sample eigenstructure for a large dimensional spiked covariance model. *Statistica Sinica* 17:1617--1642
- M. E. Tipping and C. M. Bishop (1999). Probabilistic principal component analysis. *JRSSB* 61:611--622
- Ning (2021). Spike and slab Bayesian sparse principal component analysis. *arXiv: 2102.00305*
- Ročková, V. and E. I. George (2016). Fast Bayesian factor analysis via automatic rotations to sparsity. *JASA* 111:1608–1622.
- H. Zou, T. Hastie, and Robert Tibshirani (2006). Sparse Principal Component Analysis. *JCGS* 15:265--286

Gaussian mixture model

See notes for the GM model

In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.mixture import GaussianMixture


mouse = pd.read_csv('mouse.csv', sep = " ", header = None)
X = np.array([mouse[0], mouse[1]])
GM = GaussianMixture(n_components=3, random_state=0).fit(np.transpose(X))
```

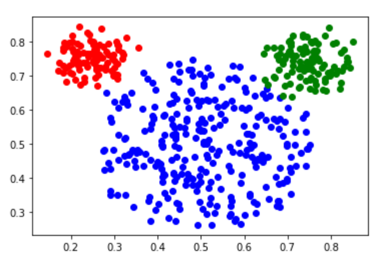
In [2]:
```
GM_predict = GM.predict(np.transpose(X))
```

In [3]:
```
mouse_GM_pred = np.transpose(np.array([mouse[0], mouse[1], GM_predict]))
mouse_head_GM_pred = mouse_GM_pred[mouse_GM_pred[:, 2] == 0]
mouse_EL_GM_pred = mouse_GM_pred[mouse_GM_pred[:, 2] == 1]
mouse_ER_GM_pred = mouse_GM_pred[mouse_GM_pred[:, 2] == 2]
```

In [4]:
```
# plot data with predicted label

plt.scatter(mouse_head_GM_pred[:, 0], mouse_head_GM_pred[:, 1],c='b',label=0)
plt.scatter(mouse_EL_GM_pred[:,0], mouse_EL_GM_pred[:,1], c='r',label=1)
plt.scatter(mouse_ER_GM_pred[:,0], mouse_ER_GM_pred[:,1], c='g',label=2)
```

Out[4]:
```
<matplotlib.collections.PathCollection at 0x7fc067819f40>
```



EM algorithm for Gaussian mixture model

See notes

Principal component analysis

Principal component analysis (PCA) is often used to reduce the dimensionality of a data set consisting of a large number of interrelated variables through orthogonal linear transformation. As a result the variation present in the data set can be retained as much as possible.

Recall the (thin) singular value decomposition (SVD) for $X = UDV'$. The left eigenvectors $U'U = I$ and D is a diagonal matrix containing eigenvalues and $V'V = VV' = I$.

For a dataset $x^n = (x_1, \dots, x_n)$, the q-th pricipal axes (v_j) are the q dominant eigenvectors (i.e., those associated with $\lambda_1, \dots \lambda_q$) of the sample covariance

$$S = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})'.$$

- *The q-th principal component (PCs)* is the q-th eigenvector of the covariance matrix S
- *The q-th Loadings* is $v_q \times d_q$.
- *PC scores* are the positions of each observation in this new coordinate system of principal components given by XV.

Yale Face Database

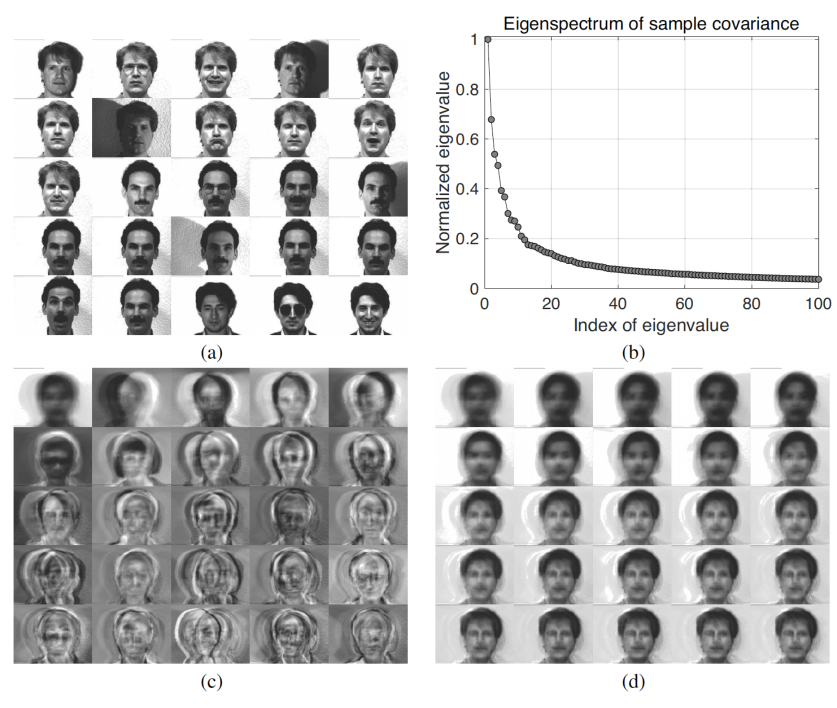


Figure 8.2 (a) Samples of face images from the Yale Face Database. (b) First 100 eigenvalues of the sample covariance matrix. (c) First 25 eigenfaces computed from the sample covariance matrix. (d) Reconstructions based on the first 25 eigenfaces plus the average face.

(Source: P239 of HDS)

Probabilistic principal component analysis and factor analysis

Consider the model

$$x_i = \mu + \theta w_i + \sigma^2 \varepsilon_i,$$

where $\theta \in \mathbb{R}^{p\times r}$ is the loadings matrix (i.e., $\theta = VD$), $w_i \overset{\text{i.i.d}}{\sim} N(0, I_r)$, and $\varepsilon_i \overset{\text{i.i.d}}{\sim} N(0, I_p)$.

One can check that $x_i \sim N(\mu, \Sigma)$, $\Sigma = \theta\theta' + \sigma^2 I_p$. The p-th eigenvalue of Σ is $\|\theta_{\cdot p}\|^2 + \sigma^2$ and p-th eigenvector is $\frac{\theta_{\cdot p}}{\|\theta_{\cdot p}\|}$. When $r < p$, there are r "spikes" $(d_1^2, \dots, d_r^2)$ in the spectrum of Σ, the covariance matrix is called spiked-covariance matrix. The model is then known as the spiked-covariance model.

How to estimate θ and σ^2?

Factor analysis

Consider the model

$$x_i = \mu + \beta w_i + \sigma^2 \varepsilon_i,$$

where $\beta \in \mathbb{R}^{p\times p}$ are the factor loadings matrix (i.e., $\theta = VDO'$, $O'O = I_r$), $w_i \overset{\text{i.i.d}}{\sim} N(0, I_p)$, and $\varepsilon_i \overset{\text{i.i.d}}{\sim} N(0, \Psi)$.

Thus, $x_i \sim N(\mu, \beta\beta' + \Psi)$

Difference between PCA and FA

- PCA asserts that all variance in a data set is common variance but FA does not
- PCA is used to decompose the data into a smaller number of orthogonal components; FA is used to understand the underlying 'cause' which these factors (latent or constituents) capture much of the information of a set of variables in the dataset data.
- The aim of PCA is to explain the variance while that of FA is to explain the covariance between the variables.

Read more here and here

High-dimensional setting

In the classical setting $n \gg p$, the sample covariance matrix $\hat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n} x_i x_i'$ is an unbiased estimator. Consider the ℓ_2-norm $\|\hat{\Sigma} - \Sigma\|_2$, the largest eigenvalue of $\hat{\Sigma} - \Sigma$, converges to zero almost surely as $n \to \infty$.

Question: what happens when $p/n = \alpha \in (0, 1)$?

In [5]:
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(2022)
n = 4000
d = 800
alpha = d/n
mean = np.zeros(d)
cov = np.identity(d)
x = np.random.multivariate_normal(mean, cov, n)
```

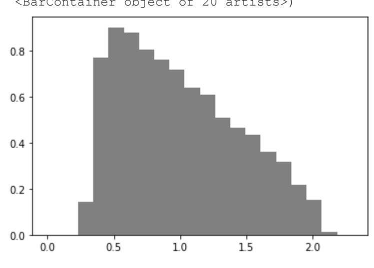
In [6]:
```
x.shape
```

Out[6]:
```
(4000, 800)
```

In [7]:
```
sample_cov = x.T @ x / n
eigen_val, eigen_vec = np.linalg.eig(sample_cov)
```

In [8]:
```
plt.hist(eigen_val, bins = 20, range = (0, 2.3), density = True, color = "gray")
```

Out[8]:
```
(array([0.        , 0.        , 0.14130435, 0.77173913, 0.90217391,
        0.88043478, 0.80434783, 0.76086957, 0.7173913 , 0.64130435,
        0.60869565, 0.51086957, 0.4673913 , 0.43478261, 0.35869565,
        0.31521739, 0.2173913 , 0.15217391, 0.01086957, 0.        ]),
 array([0.   , 0.115, 0.23 , 0.345, 0.46 , 0.575, 0.69 , 0.805, 0.92 ,
        1.035, 1.15 , 1.265, 1.38 , 1.495, 1.61 , 1.725, 1.84 , 1.955,
        2.07 , 2.185, 2.3  ]),
 <BarContainer object of 20 artists>)
```



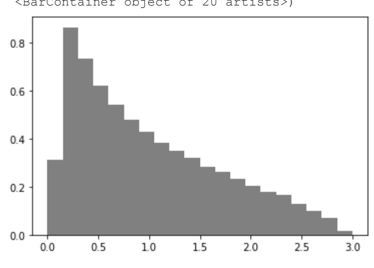
In [9]:
```
# set alpha = 0.5

n = 4000
d = 2000
mean = np.zeros(d)
cov = np.identity(d)
x = np.random.multivariate_normal(mean, cov, n)
```

In [10]:
```
sample_cov = x.T @ x / n
eigen_val, eigen_vec = np.linalg.eig(sample_cov)
```

In [11]:
```
plt.hist(eigen_val, bins = 20, range = (0, 3), density = True, color = "gray")
```

Out[11]:
```
(array([0.31      , 0.86333333, 0.73333333, 0.62      , 0.54      ,
        0.47666667, 0.43      , 0.38333333, 0.35      , 0.32      ,
        0.28333333, 0.26      , 0.23333333, 0.20333333, 0.18      ,
        0.16666667, 0.12666667, 0.1       , 0.07      , 0.01666667]),
 array([0.  , 0.15, 0.3 , 0.45, 0.6 , 0.75, 0.9 , 1.05, 1.2 , 1.35, 1.5 ,
        1.65, 1.8 , 1.95, 2.1 , 2.25, 2.4 , 2.55, 2.7 , 2.85, 3.  ]),
 <BarContainer object of 20 artists>)
```



In Ch 6 of HDS, it provides an upper bound for the maximum eigenvalue $\gamma_1(\hat{\Sigma})$ given by

$$P(\gamma_1(\hat{\Sigma}) \geq (1 + \sqrt{p/n} + \delta)^2) \leq \exp(-n\delta^2/2),$$

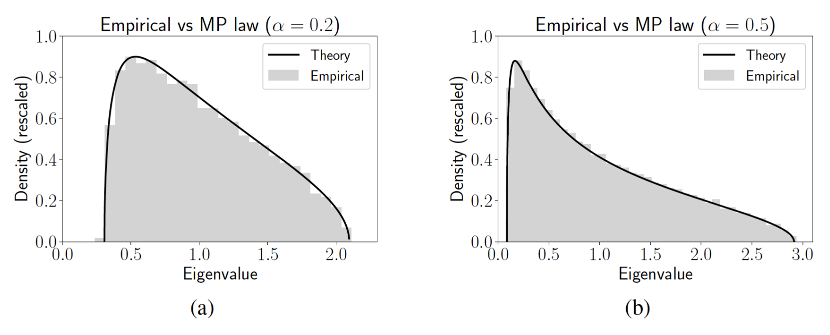
for all $\delta \geq 0$.

Marčenko-Pastur law

Let $\hat{\Sigma}$ be the sample covariance matrix given above, denote $\gamma(\hat{\Sigma}) \in \mathbb{R}^p$ be the vector of eigenvalues of $\hat{\Sigma}$, suppose $p/n \to \alpha \in (0, 1)$, then

$$f_{MP}(\gamma) \propto \sqrt{\frac{(t_1(\alpha) - \gamma)(\gamma - t_2(\alpha))}{\gamma}},$$

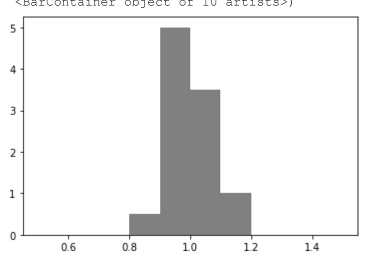
where $t_1(\alpha) = \left(1 - \sqrt{\alpha}\right)^2$ and $t_2(\alpha) = \left(1 + \sqrt{\alpha}\right)^2$, and f_{MP} is supported on the interval $[t_1(\alpha), t_2(\alpha)]$.



In [46]:
```
# set alpha = 0.5

n = 4000
d = 20
mean = np.zeros(d)
cov = np.identity(d)
x_low = np.random.multivariate_normal(mean, cov, n)
sample_cov = x_low.T @ x_low / n
eigen_val, eigen_vec = np.linalg.eig(sample_cov)
plt.hist(eigen_val, range = (0.5, 1.5), density = True, color = "gray")
```

Out[46]:
```
(array([0. , 0. , 0. , 0.5, 5. , 3.5, 1. , 0. , 0. , 0. ]),
 array([0.5, 0.6, 0.7, 0.8, 0.9, 1. , 1.1, 1.2, 1.3, 1.4, 1.5]),
 <BarContainer object of 10 artists>)
```



Spiked-covariance model

The spiked-covariance model assumes the eigenvalues of $\Sigma = (\gamma_1, \dots, \gamma_r, 1, 1, \dots, 1)$, $\gamma_1 \geq \gamma_2 \geq \dots, \gamma_r > 1$. Again, we assume $p/n = \alpha \in (0, 1)$.

According to Baik & Silverman (2006):

- If $1 \leq \gamma_v \leq 1 + \sqrt{\alpha}$, $p/n \to \alpha \in (0, 1)$, then

$$\hat{\gamma}_v \to (1 + \sqrt{\alpha})^2,$$

  almost surely as $n \to \infty$

- If $\gamma_v > 1 + \sqrt{\alpha}$, $p/n \to \alpha \in (0, 1)$, then

$$\hat{\gamma}_v \to \gamma_v\Big(1 + \frac{\alpha}{\gamma_v - 1}\Big),$$

  almost surely as $n \to \infty$

How about eigenvectors?

According to Debashis Paul (2007):

- If $\gamma_v > 1 + \sqrt{\alpha}$, $p/n \to \alpha \in (0, 1)$, let p_v be the v-th eigenvector associated with the eigenvalue γ_v and $\hat{p}_v$ be the estimated value, then

$$|\langle \hat{p}_v, p_v \rangle| \to \sqrt{\frac{\left(1 - \frac{\alpha}{(\gamma_v - 1)^2}\right)}{\left(1 + \frac{\alpha}{\gamma_v - 1}\right)}}$$

  almost surely as $n \to \infty$

- If $1 \leq \gamma_v \leq 1 + \sqrt{\alpha}$, $p/n \to \alpha \in (0, 1)$, let p_v be the v-th eigenvector associated with the eigenvalue γ_v and $\hat{p}_v$ be the estimated value, then

$$|\langle \hat{p}_v, p_v \rangle| \to 0,$$

  almost surely as $n \to \infty$.

This is so called the *phase transition phenomenon*.

Sparse PCA

Idea: imposing sparsity on loadings. Assume there are s non-zero coordinates in each eigenvector and the remaining $p - s$ coordinates are all 0. Typically, we need $rs\log p \ll n$ (one might can improve it a bit by $rs\log(ep/s)$.

1. 'Naive' approach

Let $Z_i = U_i D_{ii}$,

$$\hat{\beta} = arg\min_{\beta} \|Z_i - X\beta\|^2 + \text{Pen}_\lambda(\beta),$$

then obtain $V_i = \hat{\beta}/\|\hat{\beta}\|$.

1. "Self-contained" approach (Zou, Hastie, Tibshirani (2006))

Solve

$$(\hat{A}, \hat{B}) = arg\min_{A,B} \|X - XBA'\|^2 + \text{Pen}_\lambda(\beta), \tag{1}$$

$$\text{s.t.} \quad A'A = I_{r\times r} \tag{2}$$

Algorithm:

- Given A, solve B as in the regression setting
- Given B, we minimize $\|X - XBA'\|^2$ given $A'A = I_r$. That is, we compute SVD $(X'X)B = UDV'$ and let $\hat{A} = UV'$.

Other methods:

- Joint-row sparse for sparse PCA
- Sparse Probabilistic Principal Component Analysis by Guan and Dy (2009).
- Bayseian methods for sparse PCA and factor analysis [Rockova and George (2016); Ning (2021)]

Sparse PCA in action

SparsePCA is avilable in scikit-learn see here

The method is based on Zou et al (2006)'s paper, the elastic net penalty is added.

In [55]:
```
from sklearn.decomposition import SparsePCA
spca = SparsePCA(n_components = 30, ridge_alpha = 0.01)
```

In [56]:
```
n = 200
d = 50
mean = np.zeros(d)
cov = np.identity(d)
x = np.random.multivariate_normal(mean, cov, n)

spca.fit(x)
t_spca = spca.transform(x)
p_spca = spca.components_.T
```

In [57]:
```
import matplotlib.pyplot as plt

plt.imshow(p_spca)
plt.colorbar()
plt.show()
```