MI2_03_TheChantastic4

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1 MI2 - ES03: Batch preprocessing and Online PCA

1.1 The chantastic 4: Elisabeth Kress, Paola Suárez, Jianmeng Wu and Esra Zihni

```
In [1]: import numpy as np
        import matplotlib.pyplot as plt
        import scipy.linalg as LA
        %matplotlib inline
```

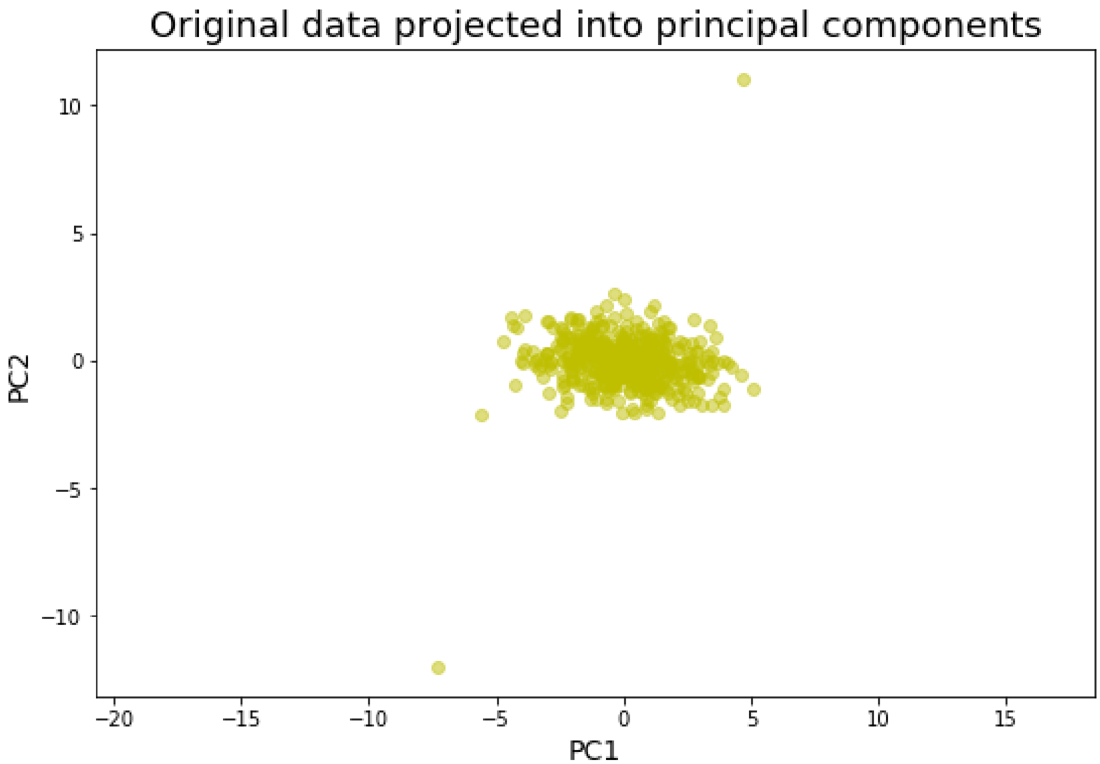
1.2 1. Preprocessing

1.2.1 1. a) Load data and compute PCA

```
In [2]: # 2d data
        filename = "pca2.csv"
        data = np.loadtxt(filename, delimiter=',', skiprows=1)

        # Zero-mean
        data -= data.mean(axis=0)
```

```
In [3]: # PCA
        cov = np.cov(data.T)
        l, w = LA.eig(cov)

        # Projection into PCs
        PCs = np.dot(w.T, data.T)
```

```
In [4]: # Plot
        plt.figure(figsize=(9,6))
        plt.scatter(PCs[0,:], PCs[1,:], alpha=0.5, c='y')
        plt.title("Original data projected into principal components", size=18)
        plt.xlabel("PC1", size=14)
        plt.ylabel("PC2", size=14)
        plt.axis('equal')
        plt.show()
```

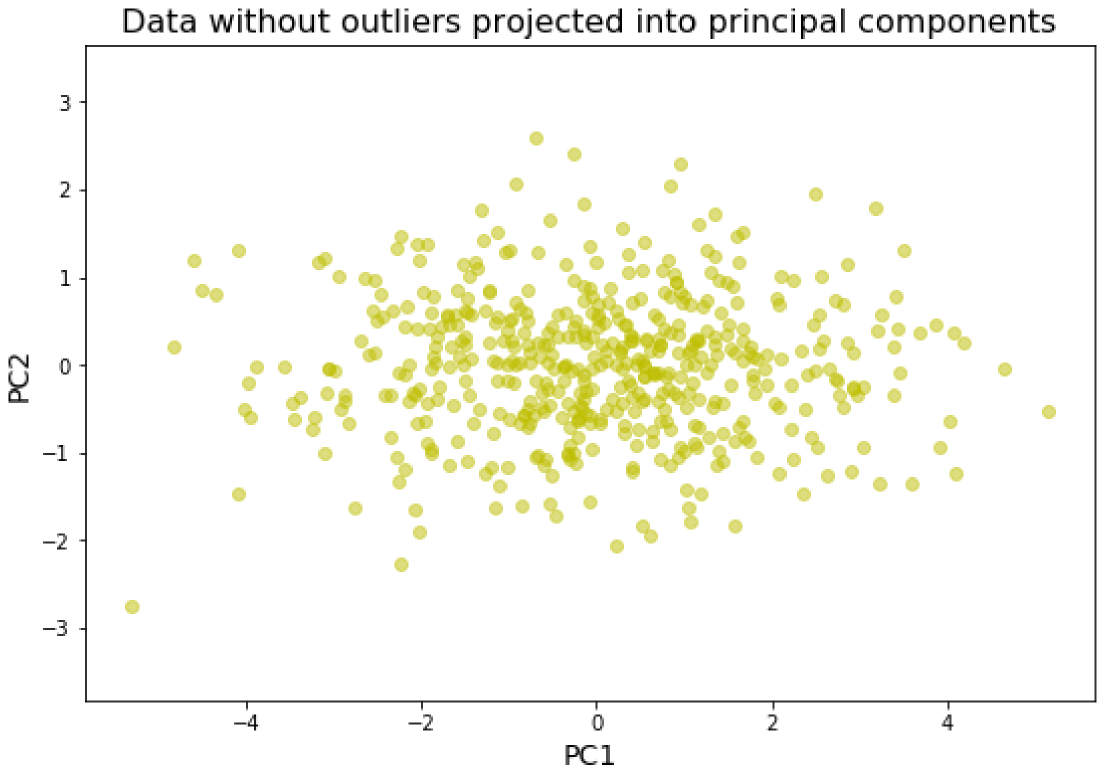


The reconstruction unveils two outliers, which contribute variance in a direction that is not aligned with the true dimensions of highest variance in the data. This means, the principal components are tilted accroding to the variance caused by the outliers.

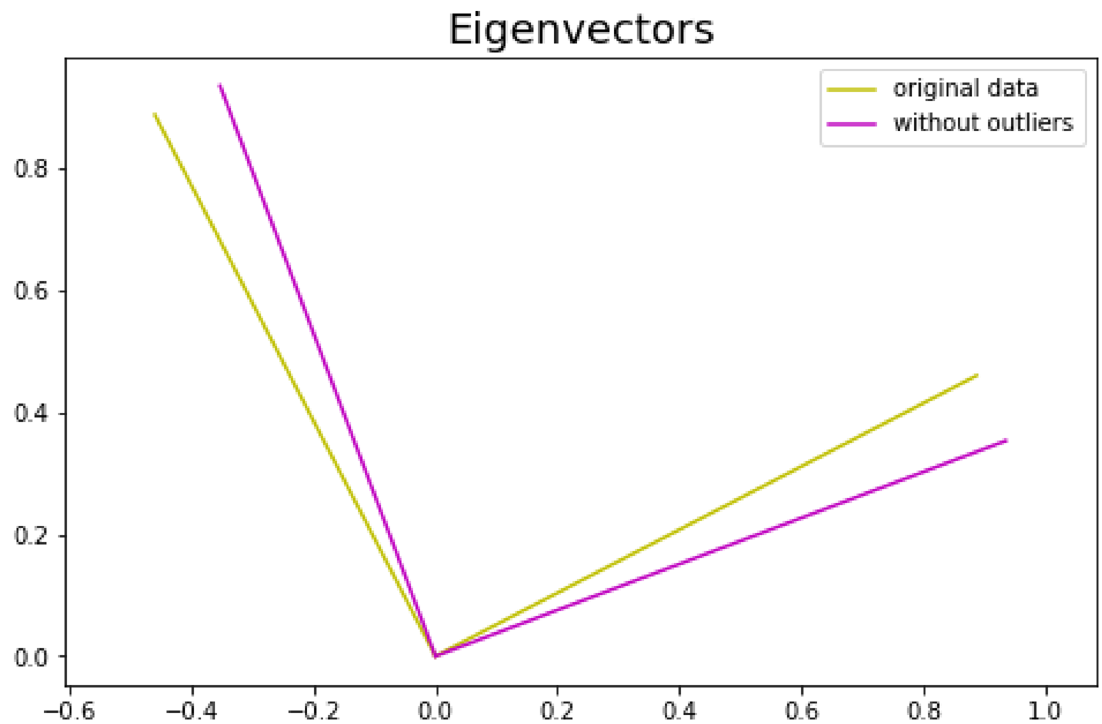
1.2.2 1. b) Remove outliers

```
In [5]: # Remove 17 and 157, i.e. 16 and 156 in python indexing.
        data_wo = np.delete(data, [16, 156], axis=0)

        data_wo -= np.mean(data_wo, axis=0)

In [6]: # PCA
        cov_wo = np.cov(data_wo.T)
        l_wo, w_wo = LA.eig(cov_wo)

        # Projection onto PCs
        PCs_wo = np.dot(w_wo.T, data_wo.T)

In [7]: # Plot
        plt.figure(figsize=(9,6))
        plt.scatter(PCs_wo[0], PCs_wo[1], alpha=0.5, c='y')
        plt.title("Data without outliers projected into principal components", size
        plt.xlabel("PC1", size=14)
        plt.ylabel("PC2", size=14)
```

```
plt.axis('equal')
plt.show()
```




```
In [8]: # plot eigenvectors
        plt.figure(figsize=(8,5))
        plt.plot([0, w[0,0]], [0, w[1,0]], 'y', label='original data')
        plt.plot([0, w[0,1]], [0, w[1,1]], 'y')
        plt.plot([0, w_wo[0,0]], [0, w_wo[1,0]], 'm', label='without outliers')
        plt.plot([0, w_wo[0,1]], [0, w_wo[1,1]], 'm')
        plt.title('Eigenvectors', size=18)
        plt.axis('equal')
        plt.legend()
        plt.show()
```



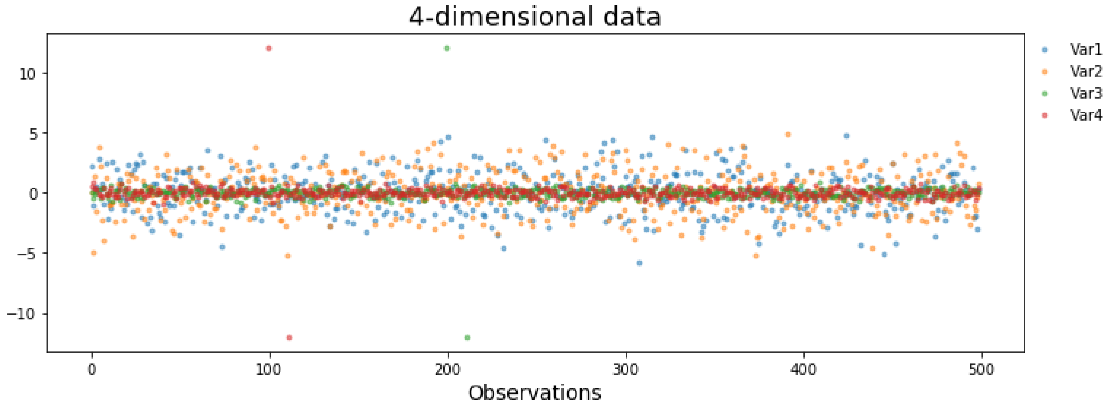
The PCs of the data without outliers are tilted as compared to the PC of the original data containing outliers. As explained above, the outliers bias the PCs in the direction in which they lie.

1.3 2. Whitening

1.3.1 2. a) Load data set and check for outliers

```
In [9]: # 4d data
        filename = "pca4.csv"
        data4 = np.loadtxt(filename, delimiter=',', skiprows=1)

        # Zero mean
        data4 -= np.mean(data4, axis=0)
```

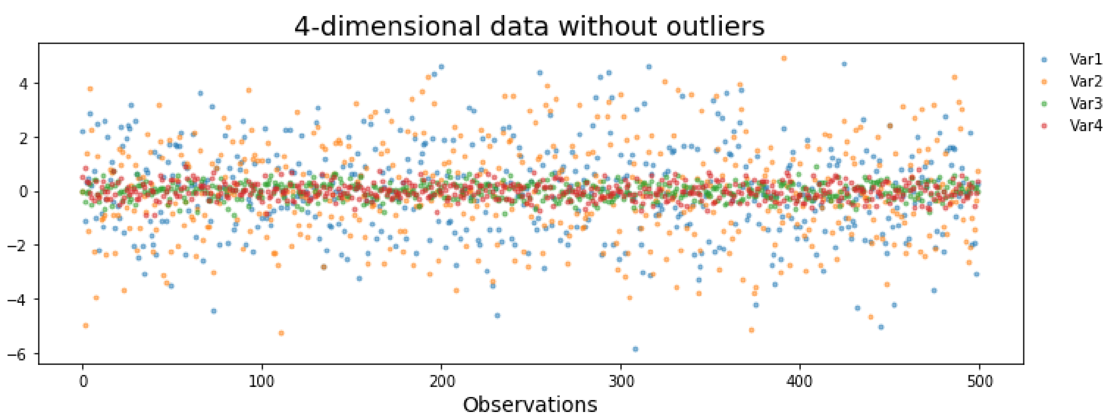
```
In [10]: # Plot to check for outliers
         plt.figure(figsize=(12,4))
         for c in range(data4.shape[-1]):
             plt.plot(data4[:,c], '.', label="Var%i" %(c+1), alpha=.5)
         plt.legend(loc=(1,0.7), frameon=False)
         plt.title('4-dimensional data', size=18)
         plt.xlabel('Observations', size=14)
         plt.show()
```



We have four outliers; to have reasonable data for PCA we will remove them.

```
In [11]: # Finda max and min, replace them with the mean
         col2, col3 = data4.copy()[:,2:].T
         max_idx = np.argmax([col2, col3], axis=1)
         min_idx = np.argmin([col2, col3], axis=1)
         col2 = np.delete(col2, [max_idx[0], min_idx[0]]) # [np.argmax(col2), np.ar
         col3 = np.delete(col3, [max_idx[1], min_idx[1]])
         mean2, mean3 = np.mean([col2, col3], axis=1)

         data4_wo = data4.copy()
         data4_wo[[max_idx[0], min_idx[0]], 2] = mean2
         data4_wo[[max_idx[1], min_idx[1]], 3] = mean3
```

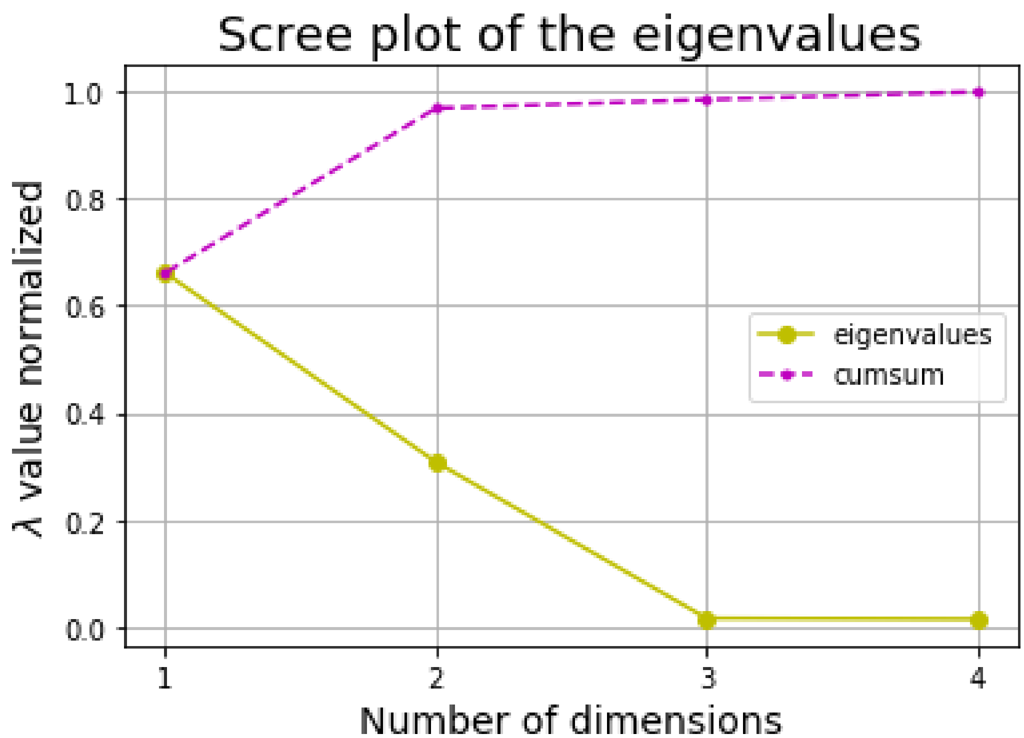
```
In [12]: # Plot again to see the result
         plt.figure(figsize=(12,4))
         for c in range(data4_wo.shape[-1]):
             plt.plot(data4_wo[:,c], '.', label="Var%i" %(c+1), alpha=.5)
         plt.legend(loc=(1,0.7), frameon=False)
         plt.title('4-dimensional data without outliers', size=18)
         plt.xlabel('Observations', size=14)
         plt.show()
```



1.3.2 2. b) PCA algorithm

```
In [13]: # PCA
         data4_wo -= data4_wo.mean(axis=0)
         cov_wo = np.cov(data4_wo.T)
         l_wo, w_wo = LA.eig(cov_wo)
         l_wo = np.real(l_wo)

         # Projection onto PCs
         PCs_wo = np.dot(w_wo.T, data4_wo.T)

         # Normalize eigenvalues
         l_wo_n = l_wo/l_wo.sum() #LA.norm(l_wo, ord=1) is equivalent
```

```
In [14]: # Scree plot
         plt.figure()
         plt.plot([1,2,3,4], l_wo_n, 'yo-', label='eigenvalues')
         plt.title("Scree plot of the eigenvalues", size=18)
         plt.xlabel("Number of dimensions", size=14)
         plt.ylabel(r"$\lambda$ value normalized", size=14)
         plt.xticks([1,2,3,4])
         plt.plot([1,2,3,4], np.cumsum(l_wo_n), 'm.--', label='cumsum')
         plt.legend(loc=7)
         plt.grid()
         plt.show()
```



Three PCs are necessary to represent the data well.

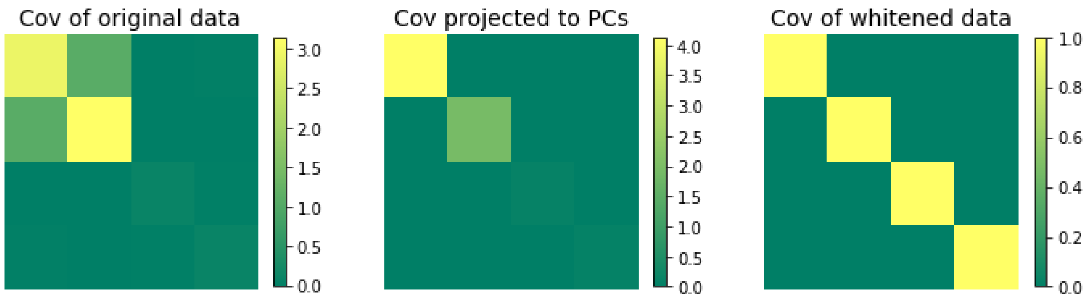
1.3.3 2. c) Whiten the data

```
In [15]: Z = np.dot(np.dot(data4_wo, w_wo), np.diag(l_wo**(-1/2))) # Don't use the
```

1.3.4 2. d) Heat plots

```
In [16]: # Covariance matrix of uncorrelated data
         cov_Z = np.cov(Z.T)

In [17]: # Plot covariance matrices
         fig, [ax1, ax2, ax3] = plt.subplots(1, 3, figsize=(12,6))
         im1 = ax1.imshow(cov_wo, cmap="summer")
         ax1.set_title("Cov of original data", size=14)
         ax1.axis("off")
         im2 = ax2.imshow(np.cov(PCs_wo), cmap="summer")
         ax2.set_title("Cov projected to PCs", size=14)
         ax2.axis("off")
         im3 = ax3.imshow(cov_Z, cmap="summer")
         ax3.set_title("Cov of whitened data", size=14)
         ax3.axis("off")
         fig.colorbar(im1, ax=ax1, shrink=0.475)
         fig.colorbar(im2, ax=ax2, shrink=0.475)
```

```
    fig.colorbar(im3, ax=ax3, shrink=0.475)
    plt.show()
```



The first heatmap shows that the first and the second variables are highly correlated. After projecting onto the PCs, all dimensions are decorrelated, but the diagonal has different values, i.e. the dimensions have different variance. Whitening the data normalizes the variances along all dimensions to 1.

1.4 3. Oja's Rule: Derivation

```
In [18]: # Load scan of derivation
         filename = "ojas_derivation.jpg"
         f = plt.imread(filename, format='jpg')
```

```
In [19]: # Show analytical solution
         plt.figure(figsize=(12,14))
         plt.imshow(f[80:1250,20:,:])
         plt.axis("off")
         plt.show()
```

Oja's Rule

3.3

$y = y(t)$ where $y = w^T x$

Hebbian Update rule with Oja Normalization

$$w_i(t+1) = \frac{w_i(t) + \varepsilon y(t) x_i(t)}{\left(\sum_{j=1}^{N} [w_j(t) + \varepsilon y(t) x_j(t)]^2\right)^{1/2}}$$

Using Taylor Expansion wrt ε around $\varepsilon = 0$

$$f(\varepsilon) = \frac{w_i(t) + \varepsilon (y(t) x_i(t))}{\left(\sum_{j=1}^{N} [w_j(t) + \varepsilon y(t) x_j(t)]^2\right)^{1/2}} \qquad f(0) = \frac{w_i(t)}{\left(\sum (w_j(t))^2\right)^{1/2}}$$

$$f'(\varepsilon) = \frac{\left(\sum_{j=1}^{N} [w_j(t) + \varepsilon y(t) x_j(t)]^2\right)^{1/2} \cdot (y(t) x_i(t)) - (w_i(t) + \varepsilon y(t) x_i(t)) \left[\frac{1}{2}\left(\sum^{N} [w_j(t) + \varepsilon y(t) x_j(t)]^2\right)^{-1/2} \cdot 2 \sum^{N} [(w_j(t) + \varepsilon y(t) x_j(t)) (y(t) x_j(t))]\right]}{\left(\left(\sum^{N} [w_j(t) + \varepsilon y(t) x_j(t)]^2\right)^{1/2}\right)^2}$$

$$f'(0) = \frac{\left(\sum_{j=1}^{N} (w_j(t))^2\right)^{1/2} \cdot y(t) x_i(t) - w_i(t) \left[\sum_{j=1}^{N} [w_j(t)]^2\right]^{-1/2} \cdot \left(\sum_{j=1}^{N} [w_j(t) \cdot (y(t) x_j(t))]\right)}{\sum_{j=1}^{N} [w_j(t)]^2}$$

$$w_i(t+1) = f(0) + f'(0)(\varepsilon - 0) + HOT$$

$$w_i(t+1) = \frac{w_i(t)}{\underbrace{\left(\sum_{j=1}^{N} w_j(t)^2\right)^{1/2}}_{2*}} + \left[\frac{y(t) x_i(t)}{\left(\sum_{j=1}^{N} w_j(t)^2\right)^{1/2}} - \frac{w_i(t) \cdot \overbrace{\sum_{j=1}^{N} w_j(t) \cdot y(t) x_j(t)}^{1*}}{\left(\sum_{j=1}^{N} [w_j(t)]^2\right)^{3/2}}\right] \varepsilon + \cancel{HOT}^{\,0}$$

$$w_i(t+1) = w_i(t) + \left[y(t) x_i(t) - \frac{w_i(t) \cdot y(t) \cdot y(t)}{1^2}\right] \varepsilon$$

$$w_i(t+1) = w_i(t) + \varepsilon y(t) [x_i(t) - w_i(t) y(t)]$$

$1*$ $y(t) = \sum_{j=1}^{N} w_j(t) x_j(t)$

$2*$ $\left(\sum_{j=1}^{N} w_j(t)^2\right)^{1/2} = 1$

with the assumption that weights normalize to 1.

1.5 4. Oja's Rule: Application

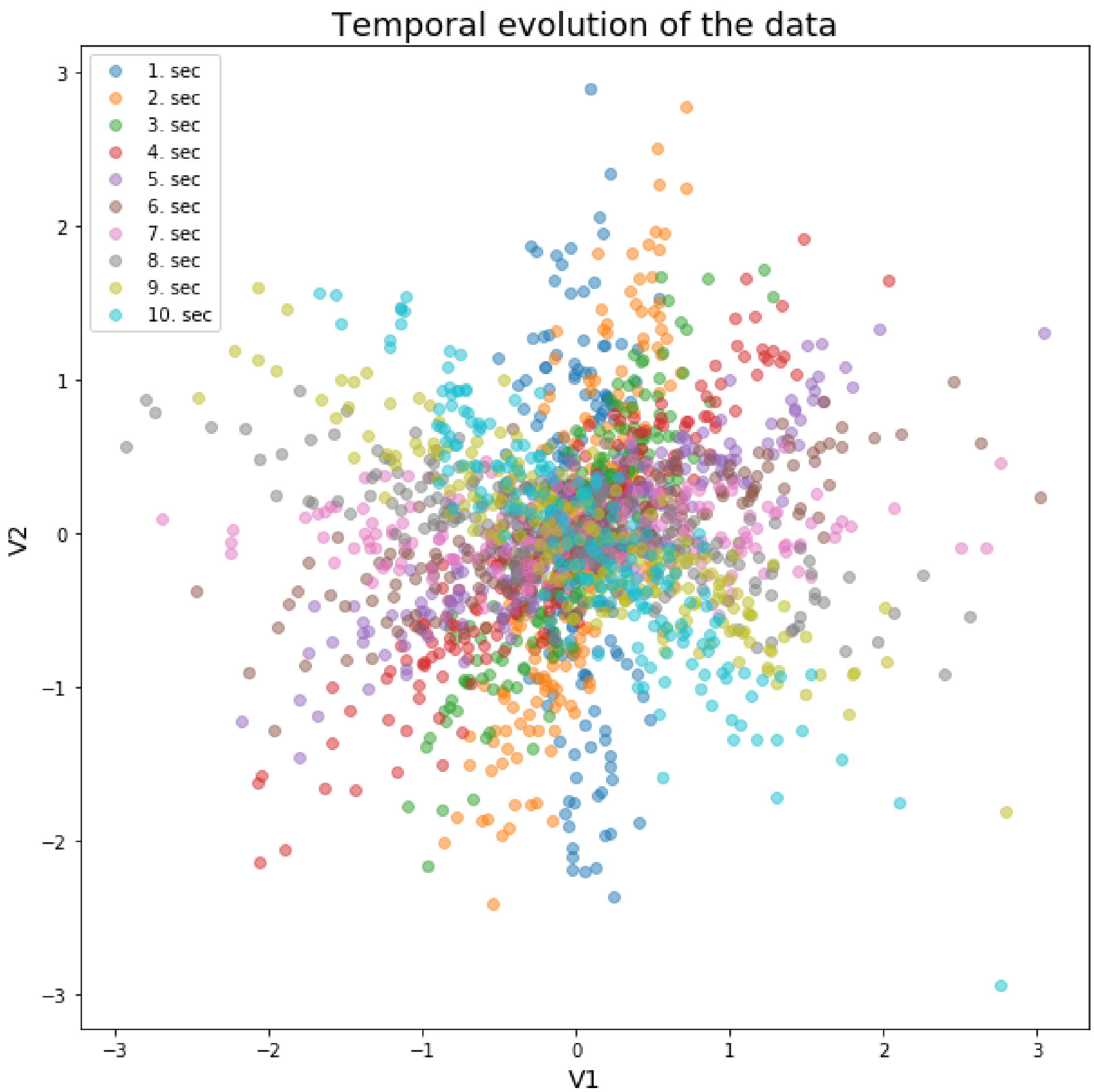
```
In [20]: # Load online data
         data_oja = np.loadtxt('data-onlinePCA.txt', delimiter=',', skiprows=1, use
```

1.5.1 4. a) Oja's Rule Scatter Plot Temporal Evolution

```
In [21]: batched_data = np.zeros((10,200,2))
         for i, j in enumerate(np.arange(0,2000,200)):
                 batched_data[i,:,:] = data_oja[j:j+200,:]
```

```
In [22]: plt.figure(figsize=(10, 10))
         for l in range(10):
```

```
    plt.plot(batched_data[l,:,0],batched_data[l,:,1],'o',alpha=0.5, label
plt.axis('equal')
plt.title("Temporal evolution of the data", fontsize=18)
plt.xlabel("V1", size=14)
plt.ylabel("V2", size=14)
plt.legend(loc='upper left')
plt.show()
```



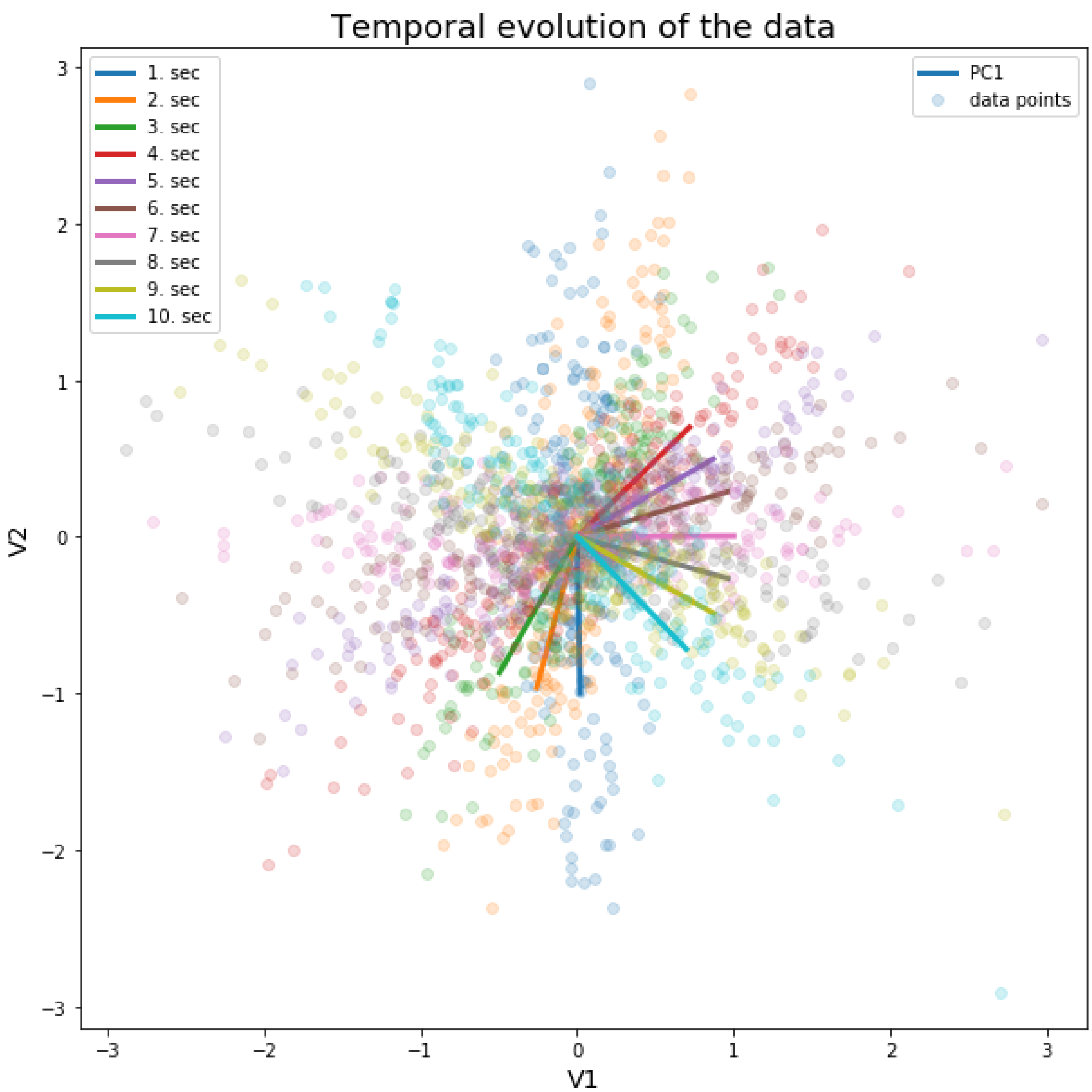
1.5.2 4. b) Determining the PCA's

```
In [23]: l_bd = np.zeros((10,2))
         cov_bd = np.zeros((10,2,2))
         w_bd = np.zeros((10,2,2))
```

```
    pc1 = np.zeros((10,2))
    for k in range(10):
        batched_data[k] -= np.mean(batched_data[k], axis=0)
        # PCA
        cov_bd[k] = np.cov(batched_data[k].T)
        l_bd[k], w_bd[k] = LA.eig(cov_bd[k])
        pc1[k]=w_bd[k,:,np.argmax(l_bd[k])]
```

```
/System/Library/anaconda/lib/python3.6/site-packages/ipykernel/__main__.py:9: Compl
```

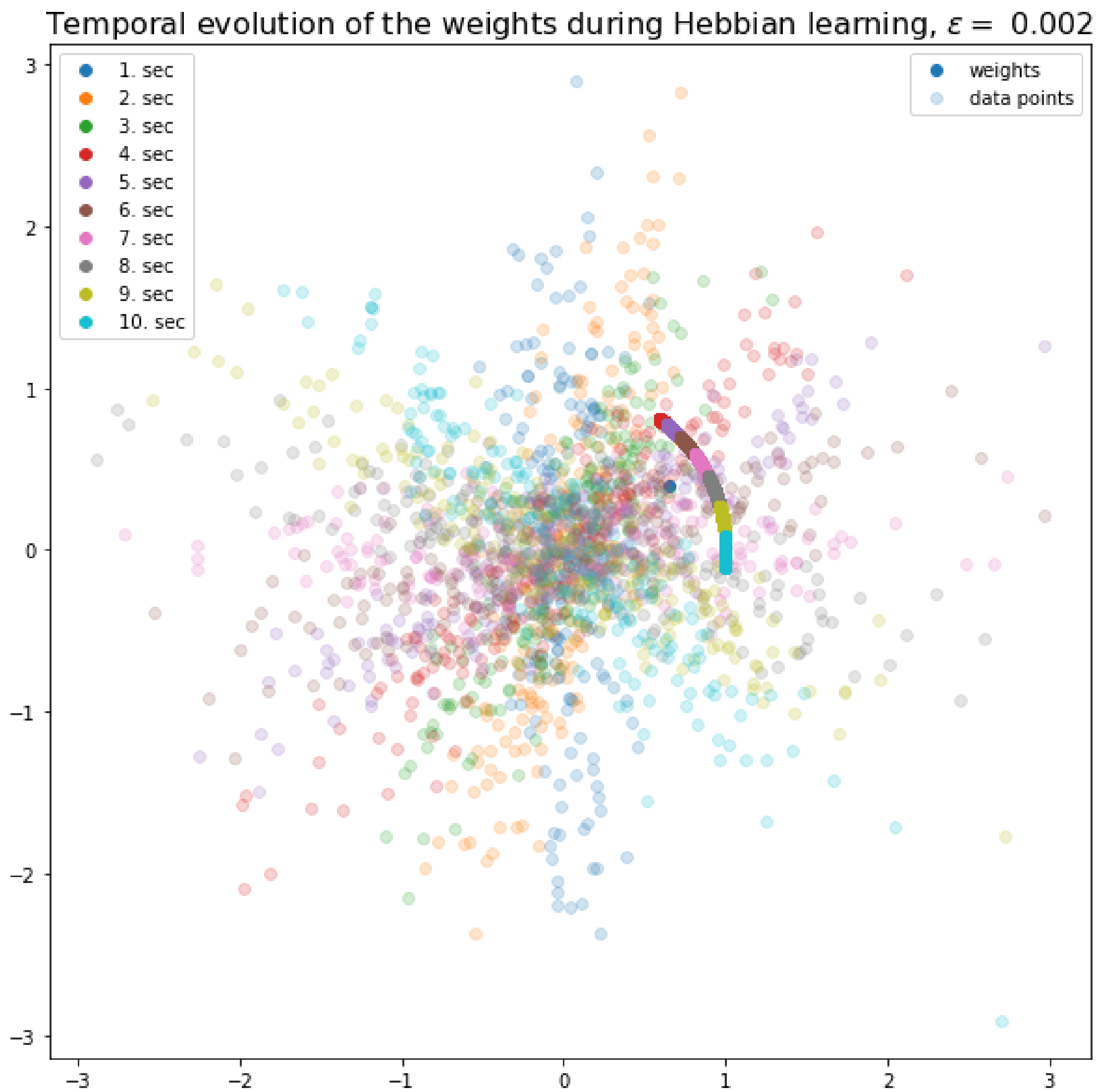
```
In [24]: plt.figure(figsize=(10, 10))
         plt.axis('equal')
         plt.title("Temporal evolution of the data", fontsize=18)
         plt.xlabel("V1", size=14)
         plt.ylabel("V2", size=14)
         plot_lines = []
         ax = plt.gca()
         for l in range(10):
             color = ax._get_lines.get_next_color()
             ln1, = plt.plot((0, pc1[l,0]),(0,pc1[l,1]),  linewidth=3.0, color=colo
             ln2, = plt.plot(batched_data[l,:,0],batched_data[l,:,1],'o', color=col

             plot_lines.append([ln1, ln2])

         legend1 = plt.legend(plot_lines[0], ['PC1', 'data points'], loc='upper rig
         plt.legend([l[0] for l in plot_lines], ['%i. sec' %(l+1) for l in range(10
         plt.gca().add_artist(legend1)
         plt.show()
```

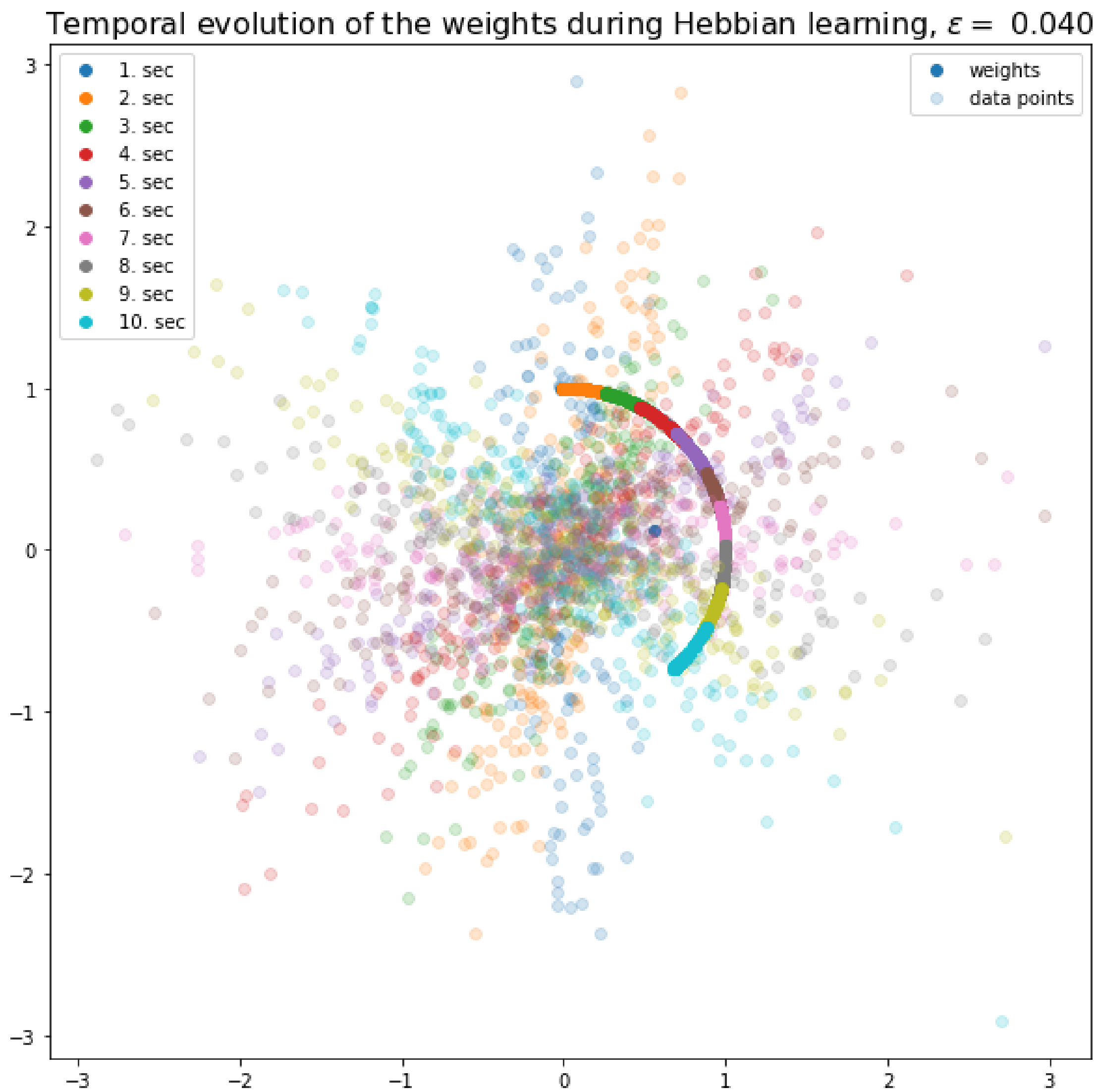


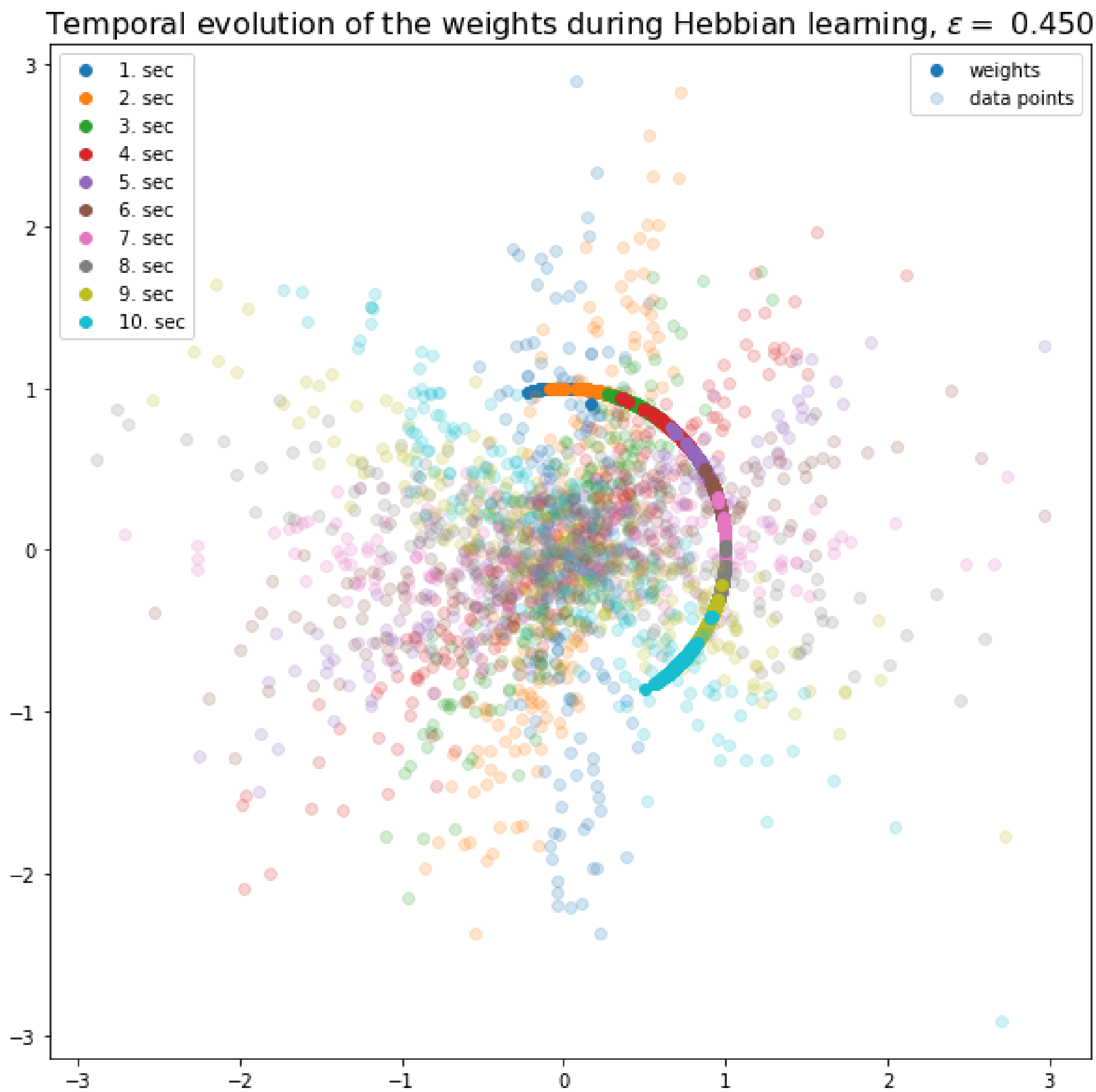
1.5.3 4. c) Implement Oja's Rule

```
In [25]: eps = [0.002, 0.04, 0.45]
         def oja(eps):
             y = np.zeros((2000,1))
             weights = np.zeros((2001,2))
             weights[0] = np.random.rand(2)
             for i in range(data_oja.shape[0]):
                 y[i] = np.dot(weights[i].T, data_oja[i])
                 weights[i+1] = (weights[i] + eps*y[i]*data_oja[i])/LA.norm(weights
             return weights

In [26]: for i in eps:
             plt.figure(figsize = (10,10))
```

```
plt.title(r'Temporal evolution of the weights during Hebbian learning,
plt.axis('equal')
plot_lines = []
ax = plt.gca()

weights = oja(i)
batched_weights = np.zeros((10,200,2))
for k, j in enumerate(np.arange(0,2000,200)):
    batched_weights[k,:,:] = weights[j:j+200,:]

for l in range(10):
    color = ax._get_lines.get_next_color()
    ln1, = plt.plot(batched_weights[l,:,0],batched_weights[l,:,1], 'o'
    ln2, = plt.plot(batched_data[l,:,0],batched_data[l,:,1],'o', color
    plot_lines.append([ln1, ln2])
plt.legend(bbox_to_anchor=(1.05, 1))
legend1 = plt.legend(plot_lines[0], ['weights', 'data points'], loc='u
plt.legend([l[0] for l in plot_lines], ['%i. sec' %(l+1) for l in rang
plt.gca().add_artist(legend1)
plt.show()
```


Temporal evolution of the weights during Hebbian learning, ε = 0.002
1. sec
2. sec
3. sec
4. sec
5. sec
6. sec
7. sec
8. sec
9. sec
10. sec
weights
data points
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3


Temporal evolution of the weights during Hebbian learning, $\varepsilon =$ 0.040
1. sec
2. sec
3. sec
4. sec
5. sec
6. sec
7. sec
8. sec
9. sec
10. sec
weights
data points



If the learning rate is too small, the weights are updated at small steps that are too slow for the temporal resolution of the data. The top figure shows that the color (which indicated time) of the weights are not aligned with the colors of the data points. The middle and the lower figures show alignment of the colors, i.e. the learning steps are well chosen.

```
In [ ]:
```