Unsupervised Learning: Dimension Reduction

Industrial AI Lab.

Dimension Reduction

- Motivation:
  - Can we describe high-dimensional data in a “simpler” way?

→ Dimension reduction without losing too much information

→Find a low-dimensional, yet useful representation of the data

Dimension Reduction

- Why dimensionality reduction?
  - insights into the low-dimensional structures in the data (visualization)
  - Fewer dimensions $\Rightarrow$ Less chances of overfitting $\Rightarrow$ Better generalization
  - Speeding up learning algorithms
    - Most algorithms scale badly with increasing data dimensionality
  - Less storage requirements (data compression)

  - Note: Dimensionality Reduction is different from Feature Selection
    - … although the goals are kind of the same
  - Dimensionality reduction is more like "Feature Extraction"
    - Constructing a small set of new features from the original features

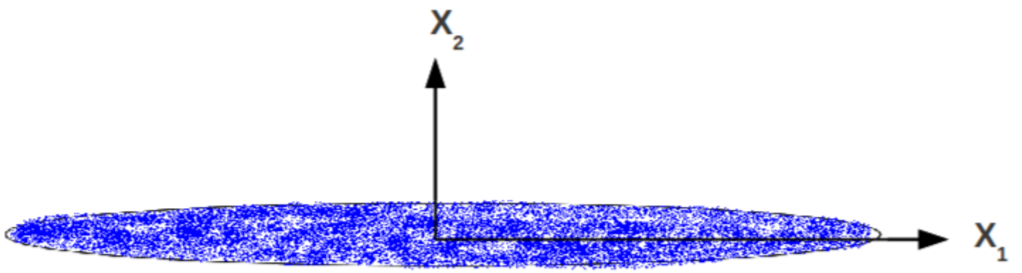
Highly Correlated Data

- How?

  idea: highly correlated data contains redundant features

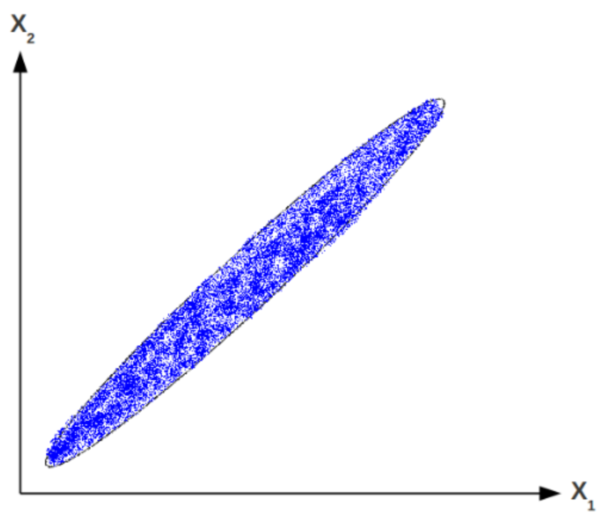
Principal Component Analysis (PCA)

- Each example x has 2 features $\{x_1, x_2\}$
- Consider ignoring the feature x_2 for each example
- Each 2-dimensional example x now becomes 1-dimensional
  $x = \{x_1\}$
- Are we losing much information by throwing away x_2?
- No. Most of the data spread is along x_1 (very little variance along x_2)



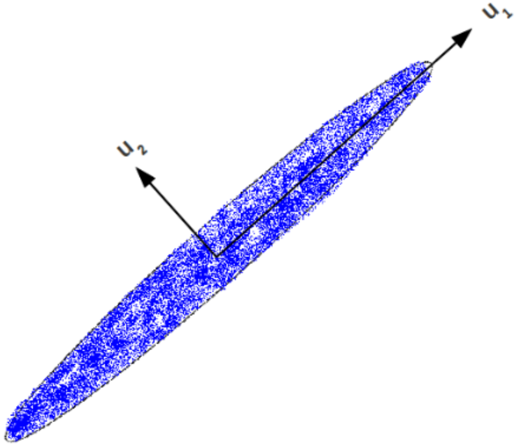
Principal Component Analysis (PCA)

- Each example x has 2 features $\{x_1, x_2\}$
- Consider ignoring the feature x_2 for each example
- Each 2-dimensional example x now becomes 1-dimensional $x = \{x_1\}$
- Are we losing much information by throwing away x_2?
- Yes, the data has substantial variance along both features (i.e., both axes)



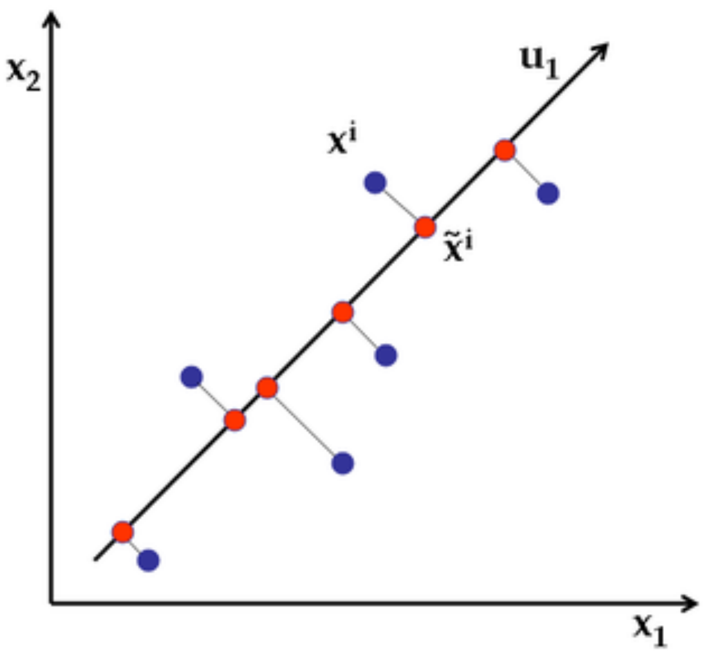
Principal Component Analysis (PCA)

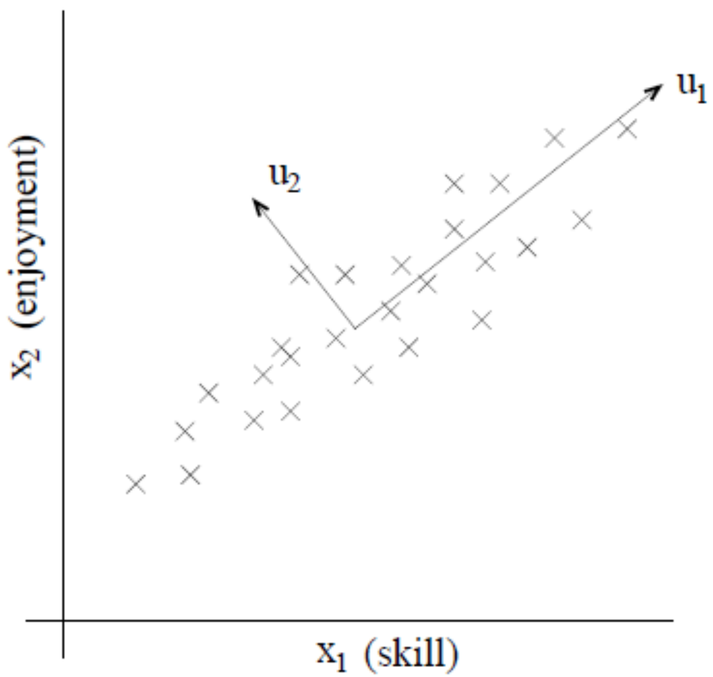
- Now consider a change of axes
- Each example x has 2 features $\{u_1, u_2\}$
- Consider ignoring the feature u_2 for each example
- Each 2-dimensional example x now become 1-dimensional
  $x = \{u_1\}$
- No. Most of the data spread is along u_1 (very little variance along u_2)



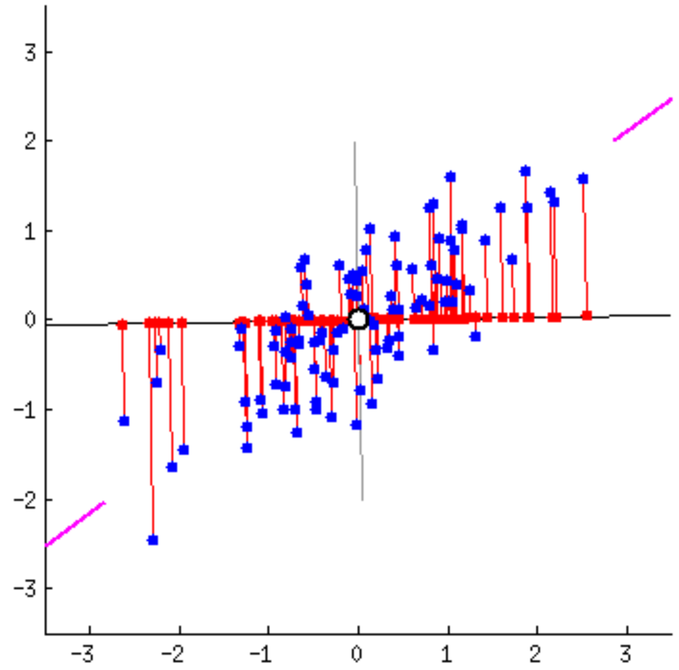
Principal Component Analysis (PCA)

- Data → projection onto unit vector $\hat{u}_1$
  - PCA is used when we want projections capturing maximum variance directions
  - Principal Components (PC): directions of maximum variability in the data
  - Roughly speaking, PCA does a change of axes that can represent the data in a succinct manner





Principal Component Analysis (PCA)



- HOW?
  1. Maximize variance (most separable)
  2. Minimize the sum-of-squares (minimum squared error)

PCA Algorithm: Pre-processing

- Given data

$$x^{(i)} = \begin{bmatrix} x_1^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}, \qquad X = \begin{bmatrix} \cdots & (x^{(1)})^T & \cdots \\ \cdots & (x^{(2)})^T & \cdots \\ & \vdots & \\ \cdots & (x^{(m)})^T & \cdots \end{bmatrix}$$

- Shifting (zero mean) and rescaling (unit variance)

1. Shift to zero mean

$$\mu = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}$$

$$x^{(i)} \leftarrow x^{(i)} - \mu \quad \text{(zero mean)}$$

2. [optional] Rescaling (unit variance)

$$\sigma_j^2 = \frac{1}{m-1} \sum_{i=1} m \left(x_j^{(i)} \right)^2$$

$$x_j^{(i)} \leftarrow \frac{x_j^{(i)}}{\sigma_j}$$

PCA Algorithm: Maximize Variance

- Find unit vector u such that maximizes variance of projections

  Note: $m \approx m - 1$ for big data

$$
\begin{aligned}
\text{variance of projected data} &= \frac{1}{m}\sum_{i=1}^{m}\left(u^T x^{(i)}\right)^2 = \frac{1}{m}\sum_{i=1}^{m}\left({x^{(i)}}^T u\right)^2 \\
&= \frac{1}{m}\sum_{i=1}^{m}\left({x^{(i)}}^T u\right)^T\left({x^{(i)}}^T u\right) = \frac{1}{m}\sum_{i=1}^{m} u^T x^{(i)} {x^{(i)}}^T u \\
&= u^T\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)} {x^{(i)}}^T\right) u \\
&= u^T S u \qquad (S = \frac{1}{m} X^T X : \text{sample covariance matrix})
\end{aligned}
$$

Maximize Variance

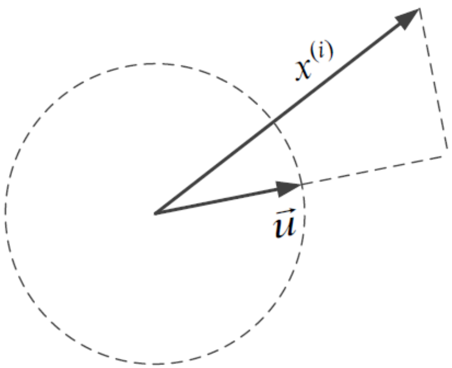
- In an optimization form

$$\begin{array}{ll} \text{maximize} & u^T S u \\ \text{subject to} & u^T u = 1 \end{array}$$

$$u^T S u = u^T \lambda u = \lambda u^T u = \lambda \quad (\text{Eigen analysis} : Su = \lambda u)$$

$$\begin{array}{l} \Longrightarrow \text{ pick the largest eigenvalue } \lambda_1 \text{ of covariance matrix } S \\ \Longrightarrow u = u_1 \text{ is the } \lambda_1' s \text{ corresponding eigenvector} \\ \Longrightarrow u_1 \text{ is the first principal component (direction of highest variance in the data)} \end{array}$$

Minimize the Sum-of-Squared Error



$$\|e^{(i)}\|^2 = \|x^{(i)}\|^2 - \left(x^{(i)T}u\right)^2$$
$$= \|x^{(i)}\|^2 - \left(x^{(i)T}u\right)^T\left(x^{(i)T}u\right)$$
$$= \|x^{(i)}\|^2 - u^T x^{(i)} x^{(i)T} u$$

$$\frac{1}{m}\sum_{i=1}^{m}\|e^{(i)}\|^2 = \frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2 - \frac{1}{m}\sum_{i=1}^{m}u^T x^{(i)} x^{(i)T} u$$
$$= \frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2 - u^T\left(\frac{1}{m}\sum_{i=1}^{m}x^{(i)}x^{(i)T}\right)u$$

Minimize the Sum-of-Squared Error

- In an optimization form

$$\text{minimize } \underbrace{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2}_{\text{constant given } x_i} - \underbrace{u^T\left(\frac{1}{m}\sum_{i=1}^{m}x^{(i)}{x^{(i)}}^T\right)u}_{\text{maximize}}$$

$$\Longrightarrow \text{maximize } u^T\left(\frac{1}{m}\sum_{i=1}^{m}x^{(i)}{x^{(i)}}^T\right)u = \max\ u^T S u$$

$$\therefore\ \text{minimize } error^2 = \text{maximize } variance$$

Dimension Reduction Method ($n \rightarrow k$)

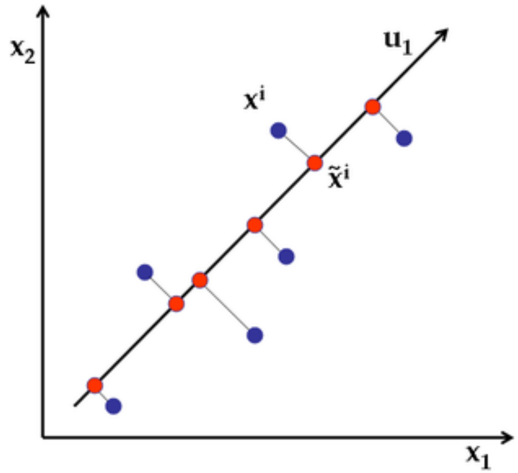
1. Choose top k (orthonormal) eigenvectors, $U = [u_1, u_2, \cdots, u_k]$
2. Project x_i onto span $\{u_1, u_2, \cdots, u_k\}$

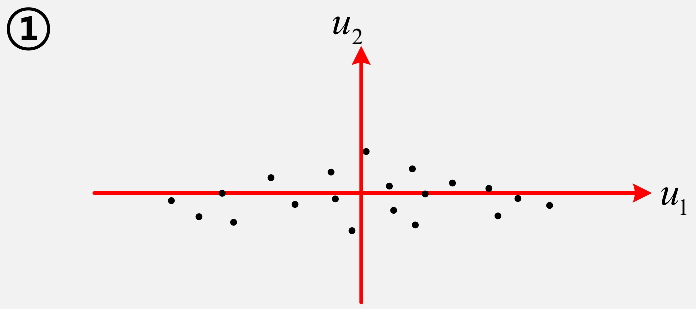
$$z^{(i)} = \begin{bmatrix} u_1^T x^{(i)} \\ u_2^T x^{(i)} \\ \vdots \\ u_k^T x^{(i)} \end{bmatrix} \quad \text{or} \quad z = U^T x$$

- $x^{(i)} \rightarrow$ projection onto unit vector $u \Longrightarrow u^T x^{(i)}$ = distance from the origin along u

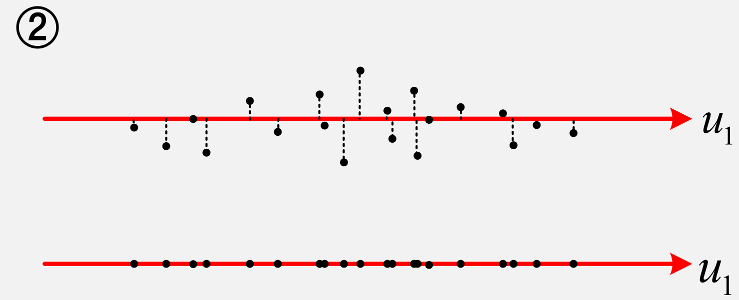
Principal Component Analysis

- Data → projection onto unit vector u



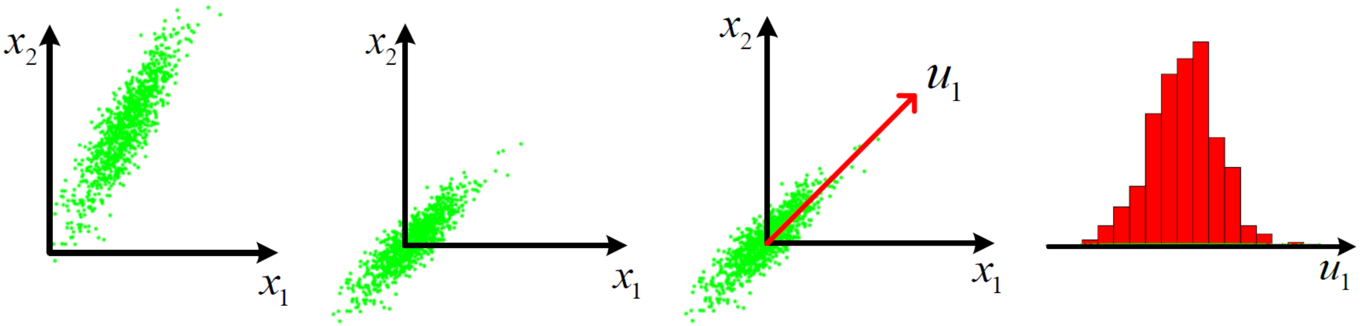


dimension 2개 선택할 경우



dimension 1개만 선택할 경우

Pictorial Summary of PCA



Pre-processing

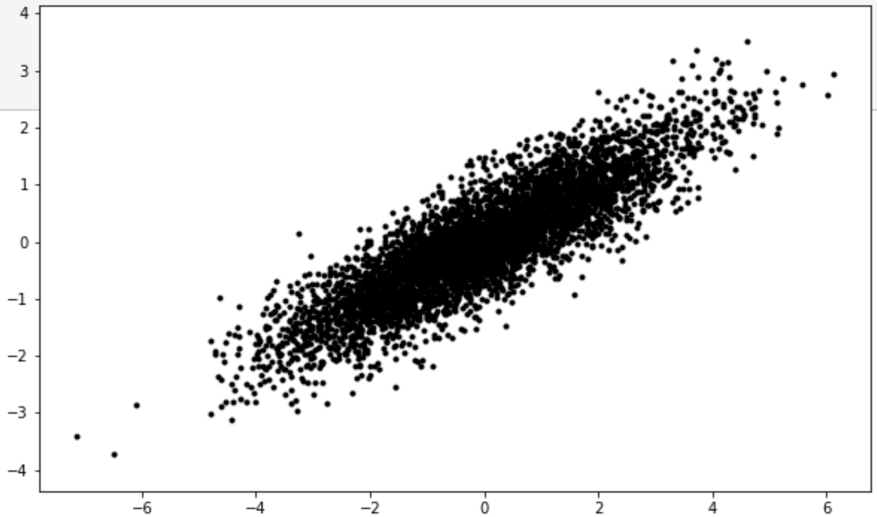
Eigenvector u

Projected
(2D→1D)

Python Codes

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import axes3d

%matplotlib inline
```

```
# data generation
m = 5000
mu = np.array([0, 0])
sigma = np.array([[3, 1.5],
                  [1.5, 1]])

X = np.random.multivariate_normal(mu, sigma, m)
X = np.asmatrix(X)

fig = plt.figure(figsize=(10, 6))
plt.plot(X[:,0], X[:,1], 'k.')
plt.axis('equal')
plt.show()
```



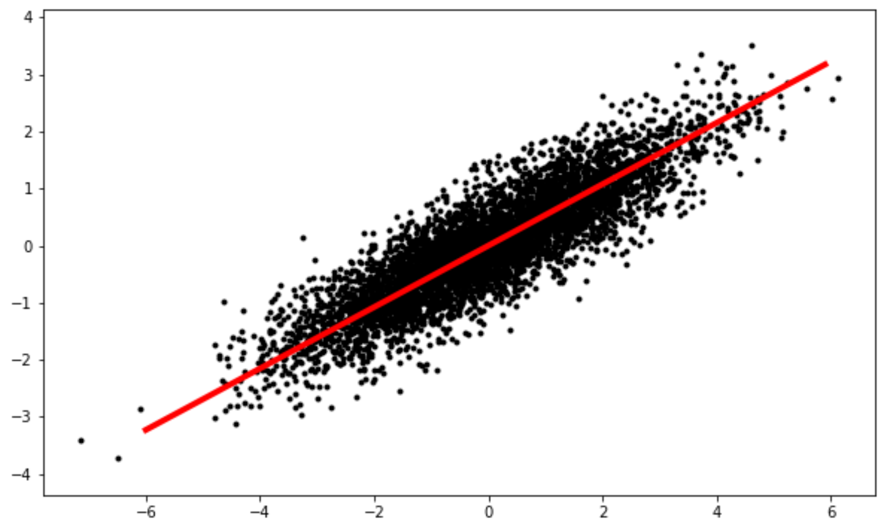
Python Codes

```
S = 1/(m-1)*X.T*X
S = np.asmatrix(S)

D, V = np.linalg.eig(S)

idx = np.argsort(-D)
D = D[idx]
V = V[:,idx]

print(D)
print(V)
```

```
[ 3.78868797  0.19209281]
[[ 0.88056479 -0.47392579]
 [ 0.47392579  0.88056479]]
```

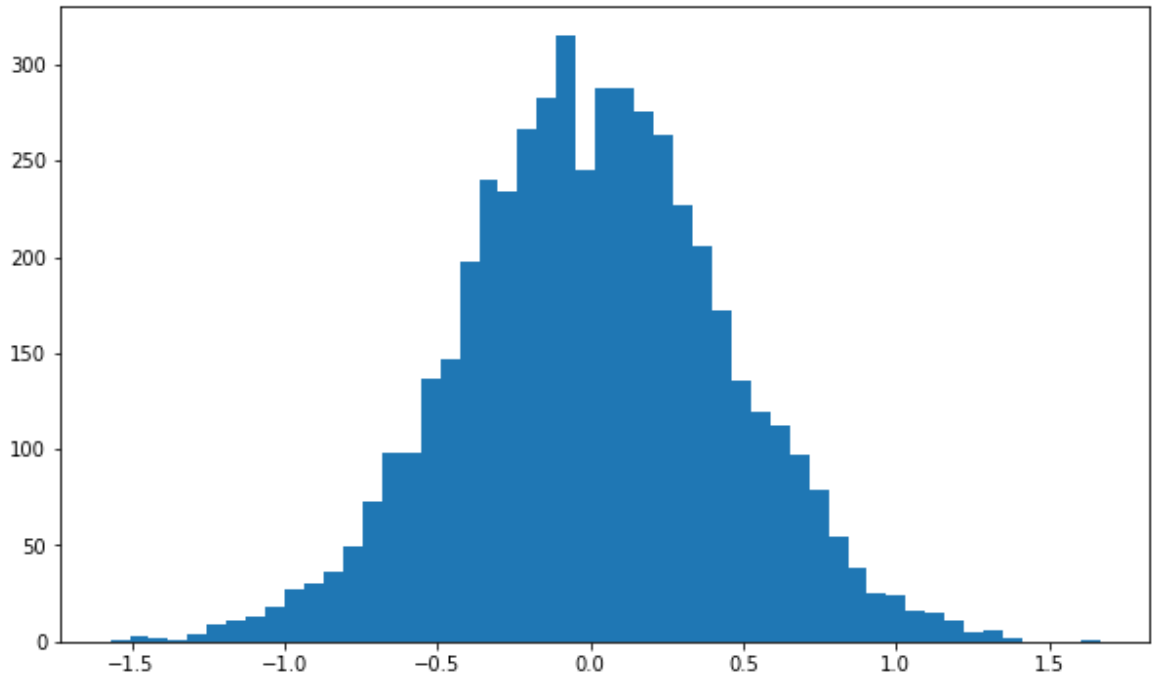
Python Codes

```
h = V[1,0]/V[0,0]
xp = np.arange(-6, 6, 0.1)
yp = h*xp

fig = plt.figure(figsize=(10, 6))
plt.plot(X[:,0], X[:,1], 'k.')
plt.plot(xp, yp, 'r', linewidth=4.0)
plt.axis('equal')
plt.show()
```



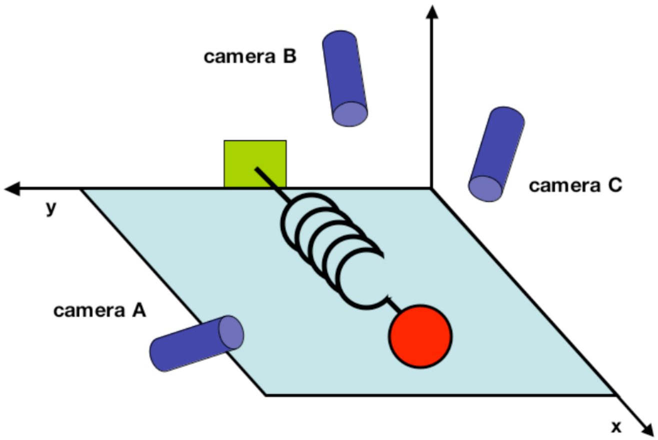
Python Codes

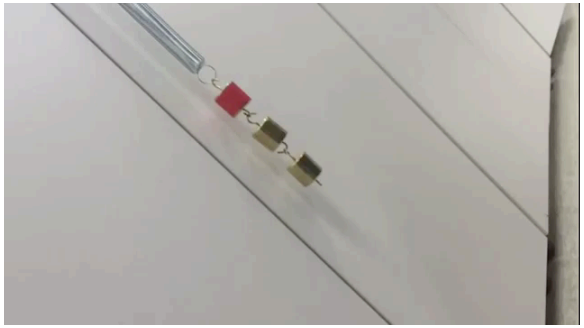
```
Z = X*V[:,1]

plt.figure(figsize=(10, 6))
plt.hist(Z, 51)
plt.show()
```

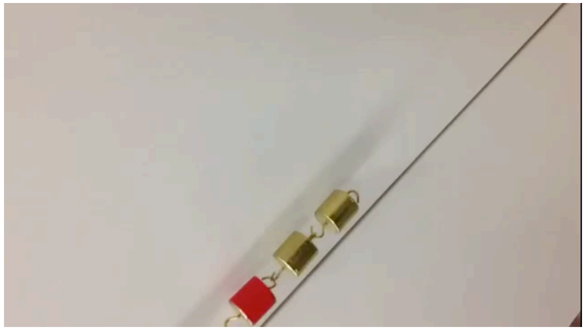


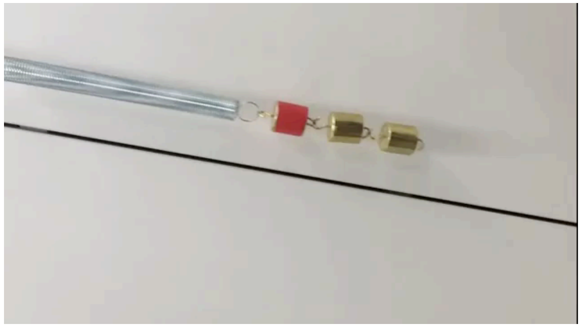
PCA Example

- Multiple video camera records of spring and mass system
- Optimal data representation
  – Find the most informative point of view



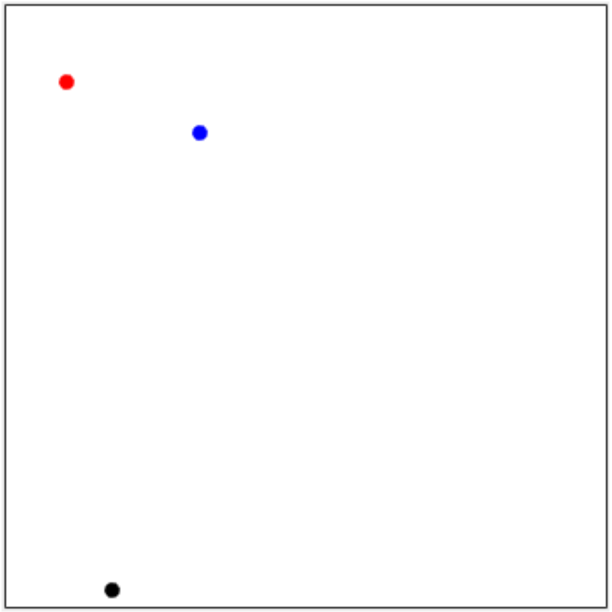






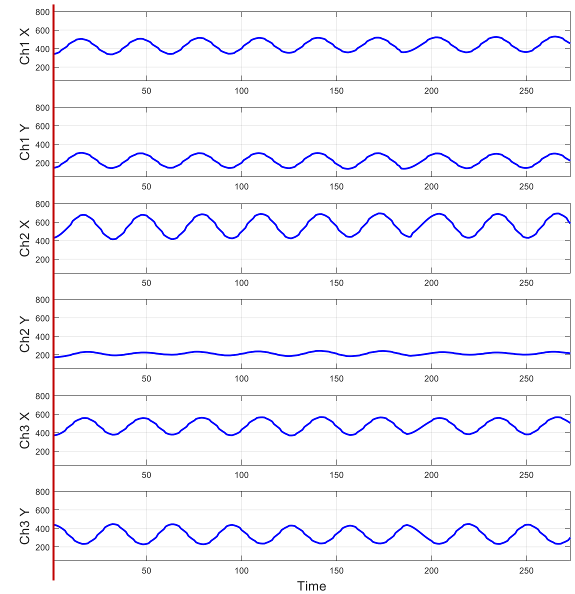
- source:
  – https://www.cs.princeton.edu/picasso/mats/PCA-Tutorial-Intuition_jp.pdf

Multivariate Time Series

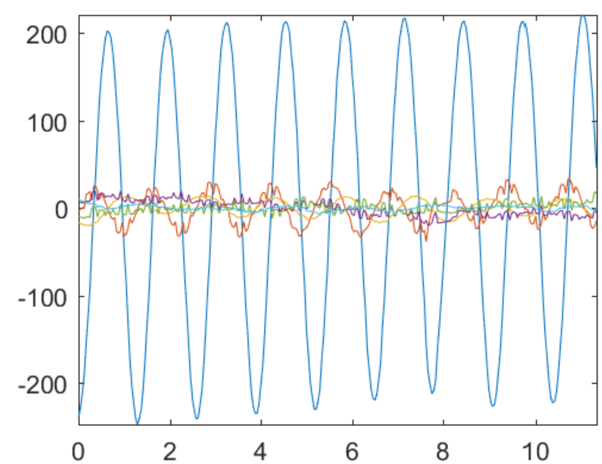


System order from
- Laws of physics or
- Data

Measured observations



Principal components



PCA Example

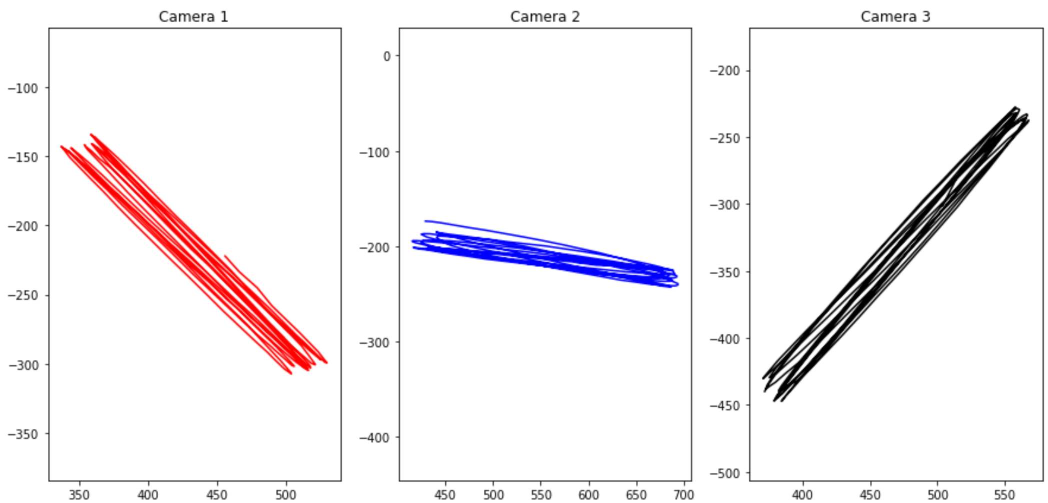
$$x^{(i)} = \begin{bmatrix} x \text{ in camera } 1 \\ y \text{ in camera } 1 \\ x \text{ in camera } 2 \\ y \text{ in camera } 2 \\ x \text{ in camera } 3 \\ y \text{ in camera } 3 \end{bmatrix}, \qquad X = \begin{bmatrix} \vdots & \vdots & & \vdots \\ (x^{(1)}) & (x^{(2)}) & \cdots & (x^{(m)}) \\ \vdots & \vdots & & \vdots \end{bmatrix}$$

```python
from six.moves import cPickle

X = cPickle.load(open('./data_files/pca_spring.pkl','rb'))
X = np.asmatrix(X.T)

print(X.shape)
m = X.shape[0]
```

```
(273, 6)
```

PCA Example

```
plt.figure(figsize=(15, 7))
plt.subplot(131)
plt.plot(X[:,0], -X[:,1],'r')
plt.axis('equal')
plt.title('Camera 1')

plt.subplot(132)
plt.plot(X[:,2], -X[:,3],'b')
plt.axis('equal')
plt.title('Camera 2')

plt.subplot(133)
plt.plot(X[:,4], -X[:,5],'k')
plt.axis('equal')
plt.title('Camera 3')

plt.show()
```



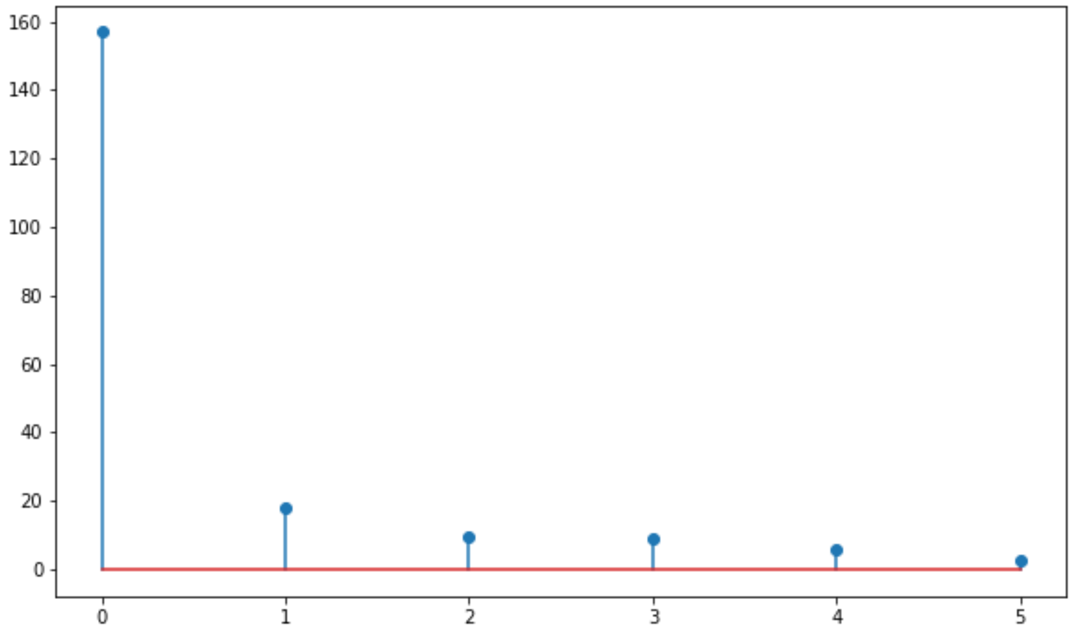
PCA Example

```
X = X - np.mean(X,axis=0)

S = 1/(m-1)*X.T*X
S = np.asmatrix(S)

D, V = np.linalg.eig(S)

idx = np.argsort(-D)
D = D[idx]
V = V[:,idx]

print(D)
print(V)
```

```
[  2.46033089e+04   3.22747042e+02   8.73851124e+01   8.19527660e+01
   3.19467195e+01   7.42861585e+00]
[[ 0.36881064  0.62298194 -0.12571821 -0.42647348  0.52121775 -0.0807439 ]
 [ 0.35632379  0.57286174  0.132303    0.59881765 -0.40143215  0.08734045]
 [ 0.58419477 -0.22610057 -0.20325551 -0.47751523 -0.58153918  0.00857804]
 [ 0.08652315 -0.02671281  0.75692234 -0.14177391 -0.06010869 -0.62861422]
 [ 0.4159798  -0.29900638  0.49374948  0.05637591  0.32442517  0.62075559]
 [-0.46389987  0.37746931  0.32963322 -0.45633202 -0.34660023  0.45308403]]
```

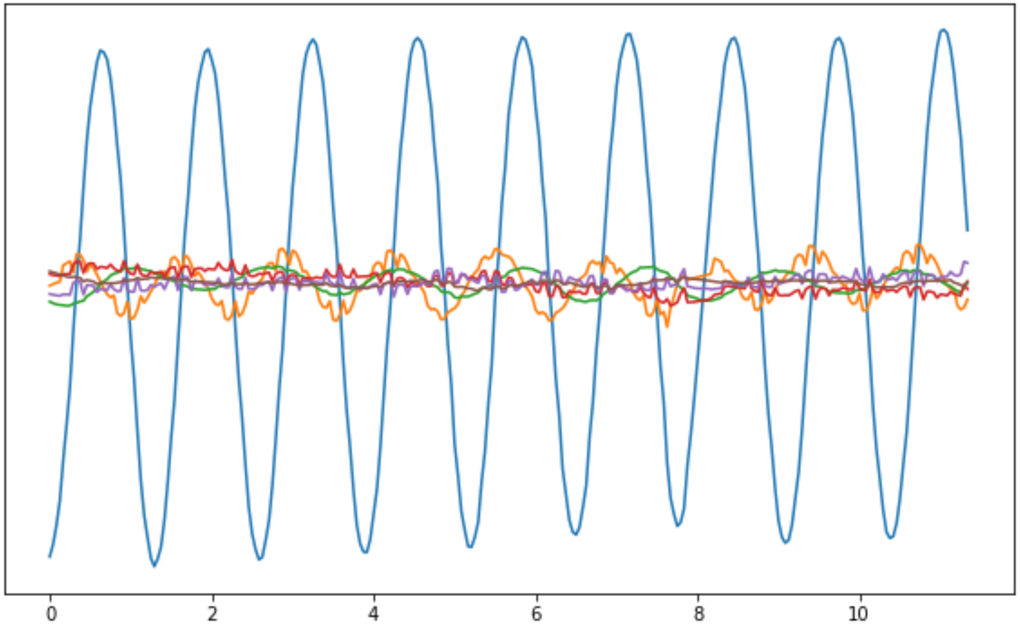
PCA Example

```
plt.figure(figsize=(10,6))
plt.stem(np.sqrt(D))
plt.show()
```



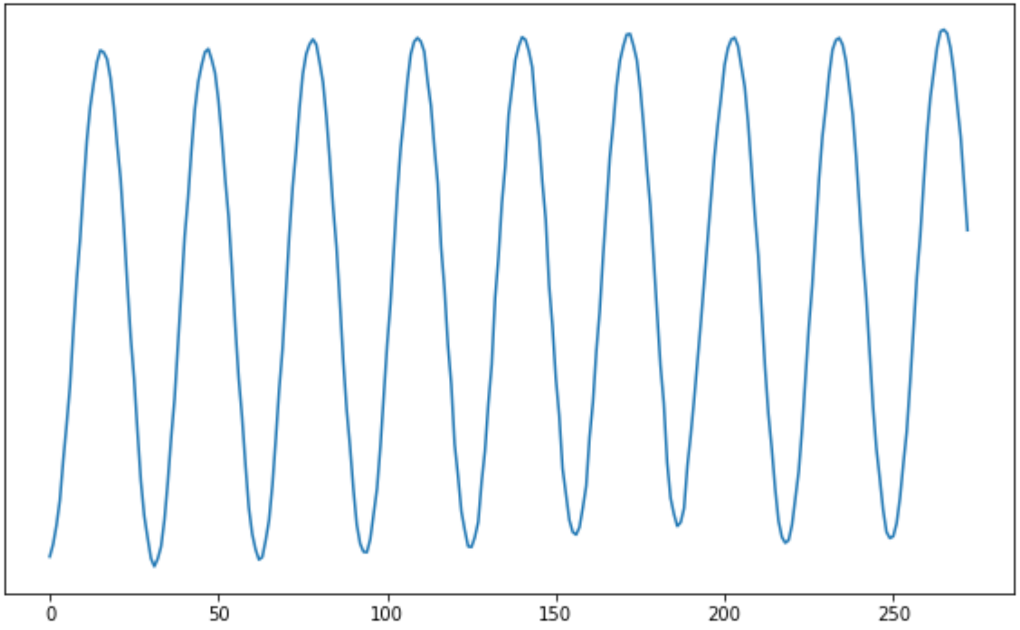
PCA Example

```
# relative magnitutes of the principal components

Z = X*V
xp = np.arange(0,m)/24

plt.figure(figsize=(10, 6))
plt.plot(xp, Z)
plt.yticks([])
plt.show()
```



PCA Example

```python
## projected onto the first principal component
# 6 dim -> 1 dim (dim reduction)
# relative magnitute of the first principal component

Z = X*V[:,0]

plt.figure(figsize=(10, 6))
plt.plot(Z)
plt.yticks([])
plt.show()
```



PCA Example

Reference: John P Cunningham & Byron M Yu, Dimensionality reduction for large-scale neural recordings, Nature Neuroscience 17, 1500–1509 (2014)