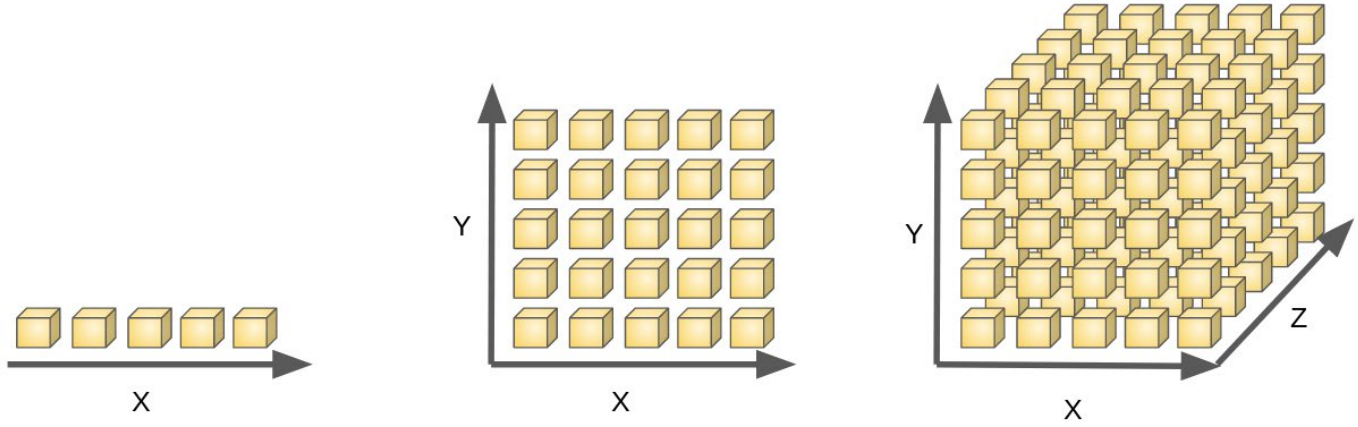
DIMENSIONALITY REDUCTION: PCA

Week12

Dimensionality Reduction

The curse of dimensionality

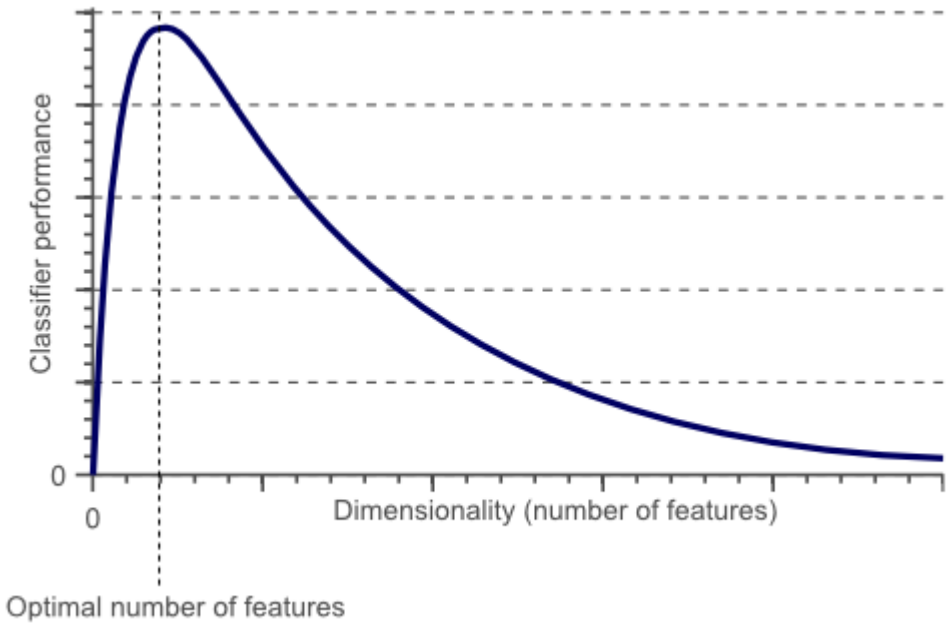
- Avoid the curse of dimensionality
  - Curse of dimensionality refers to various phenomena that arise when analyzing and organizing data in high-dimensional spaces that do not occur in low-dimensional space



  - As the dimensionality increases, we need more data to fill the space

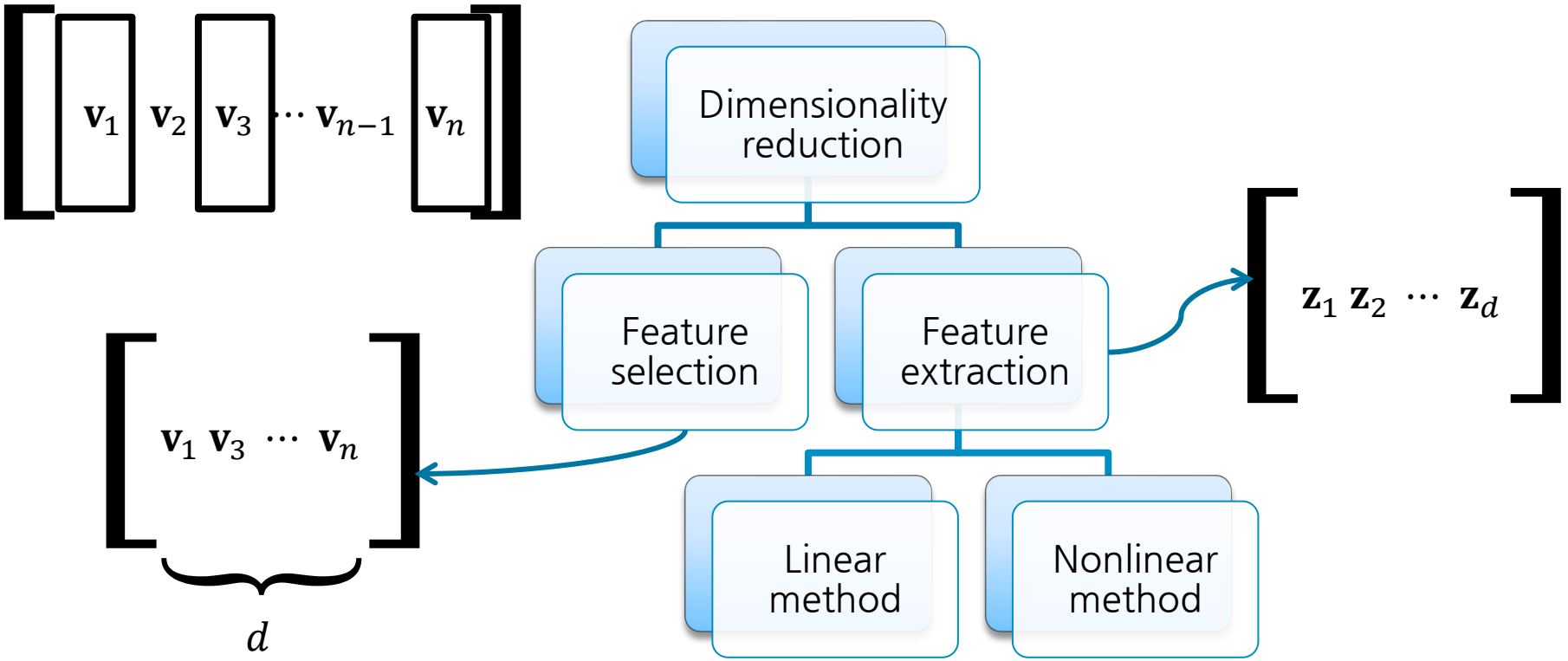
Hughes Phenomenon

- With a fixed number of training samples, the predictive power of a classifier or regressor first increases as number of dimensions/features used is increased but then decreases



Getting Rid Of The Unnecessary

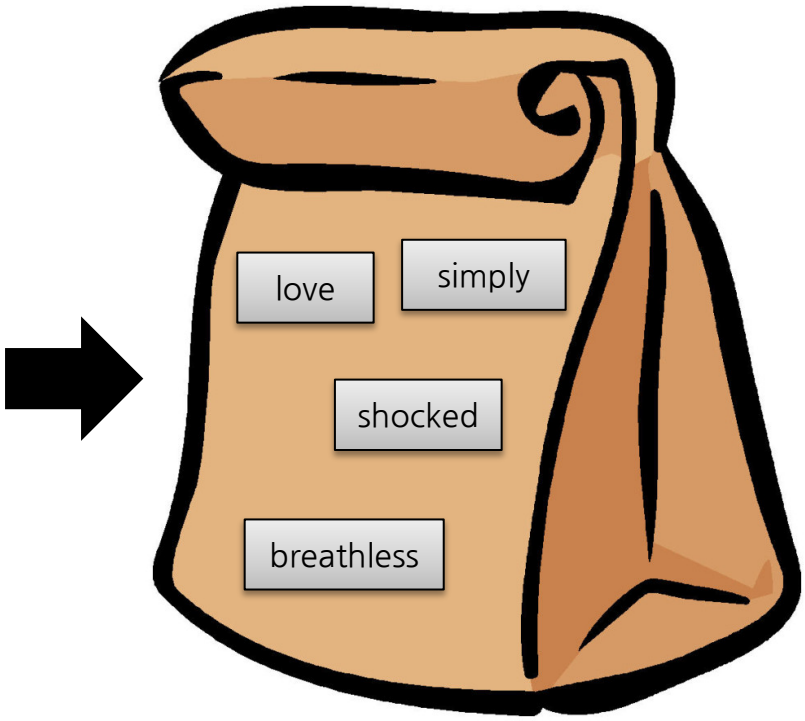
- Dimensionality reduction
  - The process of reducing the number of variables
- Hierarchy of dimensionality reduction



Example: Feature Selection

- Do you remember the bag of words representation for text data?

I simply loved this film but was shocked by the bad reviews that people gave it. To this I say to them: You seriously misunderstood the meaning of it. Although I won't reveal any real details about the meaning because I think that you should try and understand it yourself. The movie was terrific and simply breathless the whole time. I felt awestruck about how the life of one man could be so changed after an experience that Hanks went through. I say that every element of the film was perfect. And for those of you who hate Wilson, you have to understand about how human he really was to Chuck. I was amazed on how well this movie was made and think that everybody should have an experience that should cause you to take stock of your life



Example: Feature Selection

Do not stand at my grave and weep.
I am not there. I do not sleep.

Term	Frequency
do	2
not	2
stand	1
at	1
my	1
grave	1
and	1
weep	1
I	2
am	1
there	1
sleep	1

Example: Feature Selection

- Text Categorization

Politics

TRACKING TRUMP'S AGENDA | VIDEO | THE UPSHOT

Trump Is 'Not Happy' With Border Deal, but Doesn't Say if He Will Sign It

The president, who said he would have to study the deal, all but ruled out another government shutdown and emphasized that he would find "other methods" to finance a

Business | Tech | Econ | Media | Money

MARKET SNAPSHOT 11:58 PM | S&P 500 ↗ 2744.73 +1.29% | DOW INDUSTRIALS ↗ 25425.76 +1.49%

Smaller Tax Refunds Surprise Those Expecting More Relief

President Trump's tax plan promised benefits, but as returns are being filed, some frustrated people are getting smaller refunds, or even writing checks.

4h ago · By TARA SIEGEL BERNARD

CHRISTIE HEMM KLO

Technology

DEALBOOK | MARKETS | ECONOMY | ENERGY | MEDIA | TECHNOLOGY | PERSONAL TECH | ENTREPRENEURSHIP | YO

JEENAH MOON FOR THE NEW YORK TIMES

T-Mobile-Sprint Deal Gets New Scrutiny From the Left

Democratic lawmakers, empowered by their new House majority, have amplified their criticism of the deal, and two hearings are set this week.

4h ago · By CECILIA KANG

Example: Feature Selection

- Titles of the news articles

Trump Is 'Not Happy' With Border Deal, but Doesn't Say if He Will Sign It
Video

Smaller Tax Refunds Surprise Those Expecting More Relief

T-Mobile-Sprint Deal Gets New Scrutiny From the Left

Are there any irrelevant or redundant words?

Principal Component Analysis

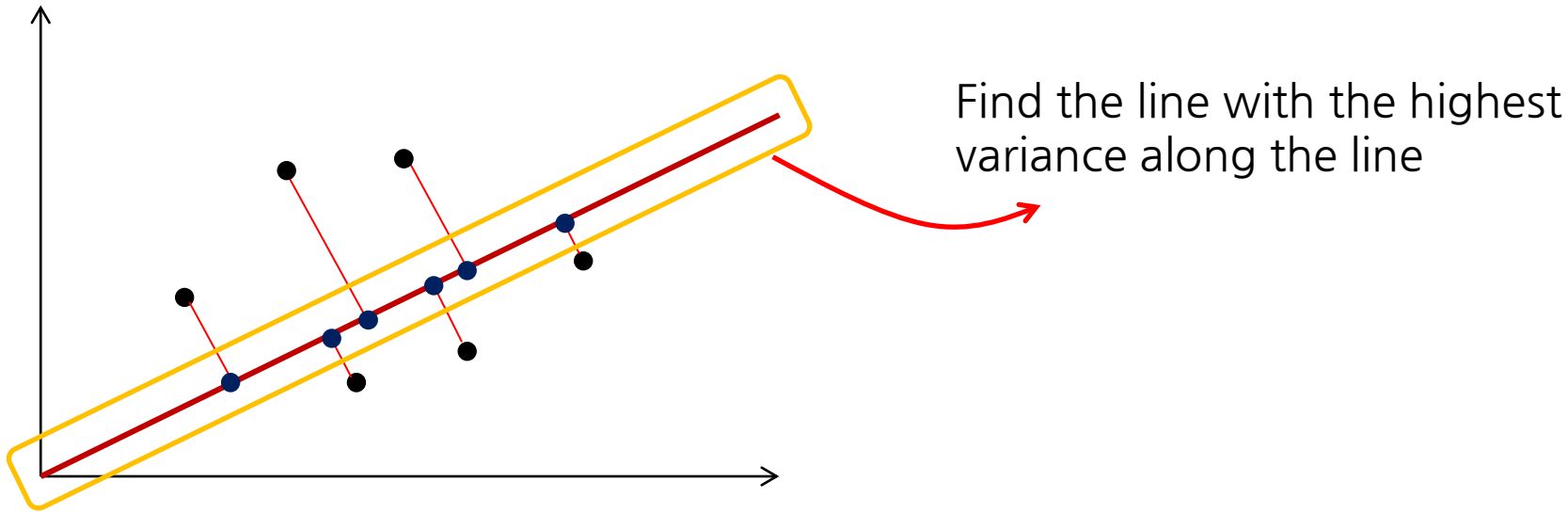
Principal Component Analysis (PCA)

- PCA is the **orthogonal transformation** to possibly correlated variables into a set of values into linearly uncorrelated variables
  - Uncorrelated variables are called principal components

- The number of principal components is less than or equal to the number of original variables
  - Even though the number of principal components are equal to the number of original variables, we select smaller number of components and then use for analysis

Principal Component Analysis (PCA)

- Criterion to find principal component is to achieve the highest variance
  - Variance of projected data samples on principal component



- First principal component has the highest possible variance
- Each succeeding component in turn has the highest variance possible and it should be orthogonal to the preceding components

Principal Component Analysis (PCA)

- Which feature is the most helpful to distinguish one house from another?

ID	Value	Area	Floors	Household
1	148	72	4	20
2	156	76	4	22
3	160	86	4	22
4	165	79	4	24
5	169	88	5	30
6	184	90	5	35

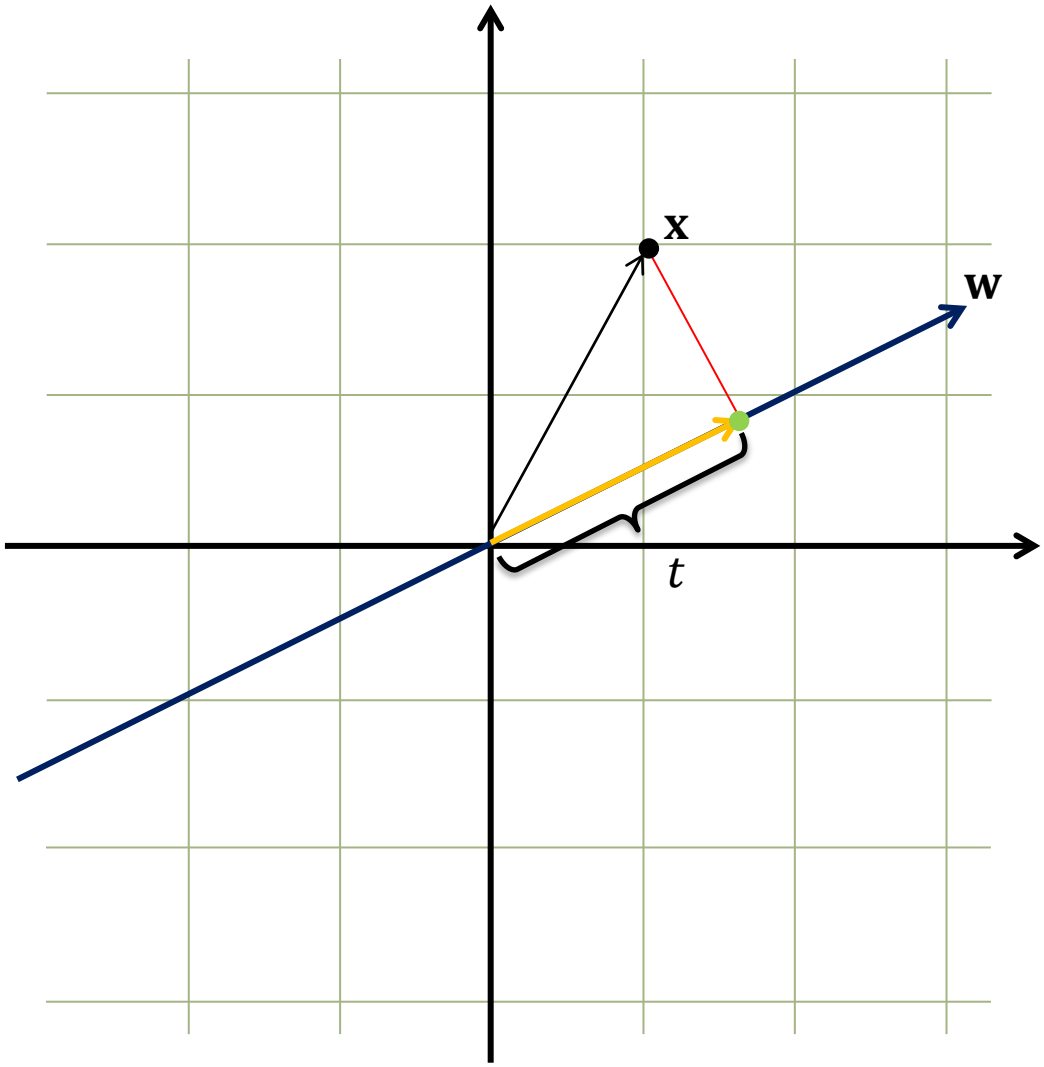
  - It's a good thing to have features with high variance, since they will be more informative and more important

→ Maximize variance

  - It's a bad thing to have highly correlated features, or high covariance, since they can be deduced from one another with little loss in information, and thus keeping them together is redundant

→ Obtain orthogonal features

※ Projection on the Line



Projected point on the line of data point $\mathbf{x}$

$t = \mathbf{w} \cdot \mathbf{x}$

Direction of line is defined as $\mathbf{w}$ and $\mathbf{w}$ is unit length vector

$\mathbf{w} = (\frac{2}{\sqrt{5}}, \frac{1}{\sqrt{5}})$

$\mathbf{x} = (1,2)$

$t = \mathbf{w} \cdot \mathbf{x} = \mathbf{w}^T\mathbf{x} = \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{5}} = \frac{4}{\sqrt{5}}$

Principal Component Analysis (PCA)

- Find first component, $\mathbf{w}_1$ for data set that each dimension has zero mean

$$\mathbf{w}_1 = \underset{\|\mathbf{w}\|=1}{\operatorname{argmax}} \sum_i (t_{1i})^2 = \underset{\|\mathbf{w}\|=1}{\operatorname{argmax}} \sum_i (\mathbf{x}_i \cdot \mathbf{w})^2$$

  - t_{1i} is the score(projected point on the first component) of i-th data point

- Define data matrix

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

$$\mathbf{X}\mathbf{w} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} \mathbf{w} = \begin{bmatrix} \mathbf{x}_1^T \mathbf{w} \\ \mathbf{x}_2^T \mathbf{w} \\ \vdots \\ \mathbf{x}_n^T \mathbf{w} \end{bmatrix}$$

Dot product $\mathbf{x}_1 \cdot \mathbf{w}$

- Rewrite $\mathbf{w}_1$

$$\mathbf{w}_1 = \underset{\|\mathbf{w}\|=1}{\operatorname{argmax}} \|\mathbf{X}\mathbf{w}\|^2 = \underset{\|\mathbf{w}\|=1}{\operatorname{argmax}} \mathbf{w}^T \mathbf{X}^T \mathbf{X} \mathbf{w}$$

Principal Component Analysis (PCA)

- Since unit vector constraint

$$\mathbf{w}_1 = \arg\max\left(\frac{\mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}}{\mathbf{w}^T\mathbf{w}}\right)$$

  - The larger $\|\mathbf{w}\|$ is, the larger $\mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}$ is
  - $\mathbf{w}^T\mathbf{w}$ is the penalty term on $\|\mathbf{w}\|$ ($\|\mathbf{w}\| = \mathbf{w}^T\mathbf{w}$)

$$\mathbf{x} = (1,2)$$
$$\mathbf{w}_1 = (1,2),\ \mathbf{w_2} = (2,4)$$
$$t_1 = \mathbf{w}_1 \cdot \mathbf{x} = {\mathbf{w}_1}^T\mathbf{x} = 1 + 4 = 5$$
$$t_2 = \mathbf{w}_2 \cdot \mathbf{x} = {\mathbf{w}_2}^T\mathbf{x} = 2 + 8 = 10$$
$$\therefore t_1^2 < t_2^2$$

- Solution of optimization problem
  - $\mathbf{w}_1$ =eigenvector of $\mathbf{X}^T\mathbf{X}$ with the largest eigenvalue
  - $\mathbf{X}^T\mathbf{X}$ is proportional to covariance matrix of data when mean of each dimension is zero

※ Covariance

- Variance of a random variable X is the expected value of the squared deviation from the mean($\mu = \mathbb{E}[X]$)

$$Var(X) = \mathbb{E}[(X - \mu)^2]$$

  - Sample variance is calculated by

$$Var(x) = \frac{\sum_{i=1}^{n}(x - \bar{x})^2}{(n-1)}$$

- Covariance is a measure of how much two random variables change together

$$Cov(X, Y) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]$$

  - Variance is the covariance of a random variable with itself

$$Var(X) = Cov(X, X)$$

  - Sample covariance is calculated by

$$cov(x, y) = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_j - \bar{y})}{n-1}$$

※ Covariance

- Covariance matrix, $\mathbf{C}$
  - Matrix whose elements correspond to possible covariance values between all the different dimensions

$$\mathbf{C} = \begin{bmatrix} cov(x_1, x_1) & cov(x_1, x_2) & \cdots & cov(x_1, x_p) \\ cov(x_2, x_1) & cov(x_2, x_2) & \cdots & cov(x_2, x_p) \\ \vdots & \vdots & & \vdots \\ cov(x_p, x_1) & cov(x_p, x_2) & \cdots & cov(x_p, x_p) \end{bmatrix}$$

  - If mean of each dimension is zero in data matrix, $\mathbf{X}$,

$$\mathbf{C} \propto \mathbf{X}^T\mathbf{X}$$

※ Eigenvector and Eigenvalue

- For some matrix $\mathbf{A}$, the vector $\mathbf{x}$ satisfying following relation is eigenvector of matrix $\mathbf{A}$

$$\mathbf{Ax} = \lambda\mathbf{x}$$

  - λ is the eigenvalue of eigenvector $\mathbf{x}$
  - The number of eigenvectors depends on matrix

- Example

$$\mathbf{A} = \begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix}$$

  - For vector $\mathbf{x} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$

$$\mathbf{Ax} = \begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 11 \\ 5 \end{bmatrix}$$

NOT eigenvector

  - For vector $\mathbf{y} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$

$$\mathbf{Ay} = \begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix}\begin{bmatrix} 3 \\ 2 \end{bmatrix} = \begin{bmatrix} 12 \\ 8 \end{bmatrix} = 4\begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

eigenvector

eigenvalue

※ Eigenvector and Eigenvalue

- How to get eigenvector and eigenvalue?

$$\mathbf{A} = \begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix}$$

  - Eigenvector and eigenvalue should satisfy $\mathbf{Ax} = \lambda\mathbf{x}$

$$\begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \lambda\begin{bmatrix} x \\ y \end{bmatrix} \rightarrow \begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} - \lambda\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 2-\lambda & 3 \\ 2 & 1-\lambda \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = 0$$

  - If there exist nontrivial solution(trivial solution=$\begin{bmatrix} x \\ y \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \end{bmatrix}$), determinant of $\begin{bmatrix} 2-\lambda & 3 \\ 2 & 1-\lambda \end{bmatrix}$ should be 0

$$(2-\lambda)(1-\lambda) - 6 = 0 \rightarrow \lambda^2 - 3\lambda + 4 = 0$$
$$\lambda = 4 \; or \; -1$$

  - When $\lambda = 4, \mathbf{x} = [3 \quad 2]^T$
  - When $\lambda = -1, \mathbf{x} = [1 \quad -1]^T$

Principal Component Analysis (PCA)

- Succeeding process
  - Subtracting preceding components from $\mathbf{X}$ → Create new data matrix

$$\widehat{\mathbf{X}}_k = \mathbf{X} - \sum_{i=1}^{k-1} \mathbf{X}\,\mathbf{w}_i\mathbf{w}_i^T$$

  - Find the principal component that extracts the maximum variance from new data matrix

$$w_k = \underset{\|\mathbf{w}\|=1}{\operatorname{argmax}} \left\|\widehat{\mathbf{X}}_k\mathbf{w}\right\|^2 = \arg\max\left(\frac{\mathbf{w}^T\widehat{\mathbf{X}}_k{}^T\widehat{\mathbf{X}}_k\mathbf{w}}{\mathbf{w}^T\mathbf{w}}\right)$$

    - Solve above equation is the also same as calculated the remaining eigenvectors of $\mathbf{X}^T\mathbf{X}$
    - $\mathbf{w_2}$ =eigenvector of $\mathbf{X}^T\mathbf{X}$ with the second largest eigenvalue

Principal Component Analysis (PCA)

- Finally,

$$\mathbf{T} = \mathbf{XW}$$

  - $\mathbf{W}$ is p-by-p matrix whose columns are the eigenvectors of $\mathbf{X}^T\mathbf{X}$ and it is called loading matrix

$$\mathbf{W} = [\mathbf{w}_1 \quad \mathbf{w}_2 \quad \cdots \quad \mathbf{w}_p]$$

  - Principal component is linear combinations of original features and transformation by loading matrix is linear transformation

- Dimensionality reduction by PCA
  - Keeping only the first l principal components (where $p > l$)

$$\mathbf{W}_l = [\mathbf{w}_1 \quad \mathbf{w}_2 \quad \cdots \quad \mathbf{w}_l]$$

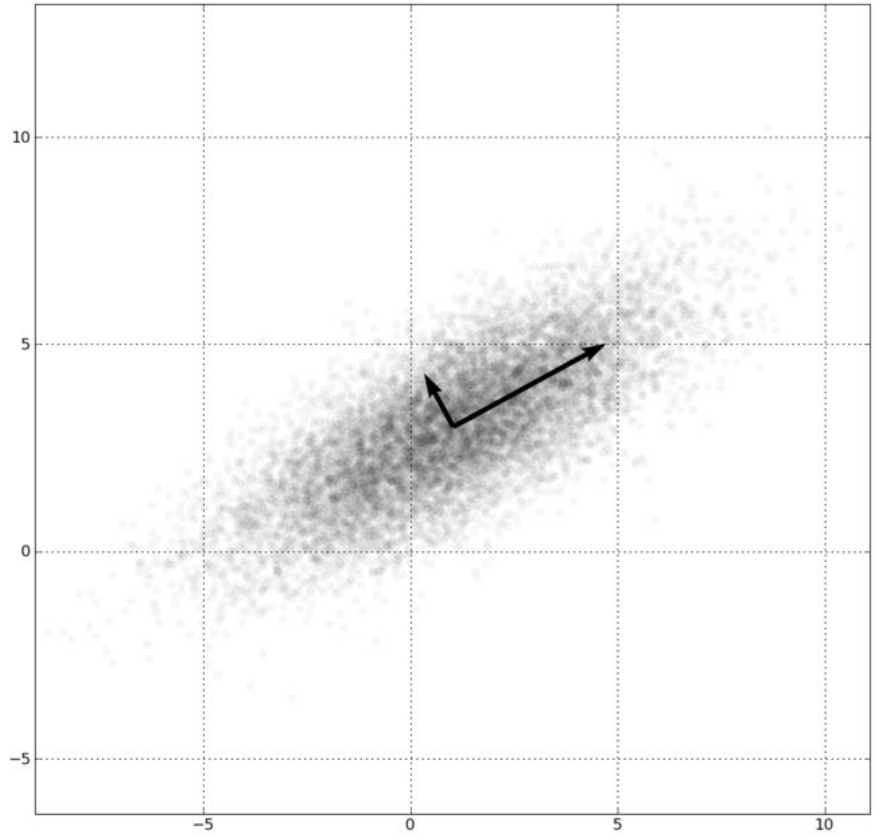
    - $\mathbf{W}_l$ is $p \times l$ matrix

- Dimension-reduced data set is obtained by truncated transformation

$$\mathbf{T}_l = \mathbf{XW}_l$$

Principal Component Analysis (PCA)

- 2-dimensional data set and its principal components



- Web applet
  - https://setosa.io/ev/principal-component-analysis/

※ Linear Combination

- If $\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_n$ are vectors and $a_1, a_2, \cdots, a_n$ are scalars, then linear combination of those vectors with those scalars as coefficient is

$$a_1\mathbf{v}_1 + a_2\mathbf{v}_2 + \cdots + a_n\mathbf{v}_n$$

- 3-dimensional vector (a_1, a_2, a_3) is linear combination of $e_1 = (1,0,0), e_2 = (0,1,0), e_3 = (0,0,1)$

$$(a_1, a_2, a_3) = (a_1, 0,0) + (0, a_2, 0) + (0,0, a_3)$$
$$= a_1(1,0,0) + a_2(0,1,0) + a_3(0,0,1) = a_1e_1 + a_2e_2 + a_3e_3$$

- Principal component $\mathbf{w} = (w_1, w_2, \ldots, w_p)$ is linear combination of unit vectors on each dimension representing by each variables

Example: PCA

- Find principal components of given data

x	2.5	0.5	2.2	1.9	3.1	2.3	2.0	1.0	1.5	1.1
y	2.4	0.7	2.9	2.2	3.0	2.7	1.6	1.1	1.6	0.9

  - Step1) substract from of the data dimensions for each dimension to have zero mean
    - $\bar{x} = 1.81, \bar{y} = 1.91$

x	0.69	-1.31	0.39	0.09	1.29	0.49	0.19	-0.81	-0.31	-0.71
y	0.49	-1.21	0.99	0.29	1.09	0.79	-0.31	-0.81	-0.31	-1.01

  - Step 2) Calculate covariance matrix of new data($\mathbf{X}^T\mathbf{X}$)

$$C = \begin{bmatrix} 0.617 & 0.615 \\ 0.615 & 0.717 \end{bmatrix}$$

Example: PCA

- Find principal components of given data

x	2.5	0.5	2.2	1.9	3.1	2.3	2.0	1.0	1.5	1.1
y	2.4	0.7	2.9	2.2	3.0	2.7	1.6	1.1	1.6	0.9

  - Step 3) Calculate the eigenvectors and eigenvalues of the covariance matrix
    - The largest eigenvalue is 1.28 and corresponding eigenvector is

$$\mathbf{w}_1 = \begin{bmatrix} -0.678 \\ -0.735 \end{bmatrix}$$

    - The second largest eigenvalue is 0.049 and corresponding eigenvector is

$$\mathbf{w}_2 = \begin{bmatrix} -0.735 \\ 0.678 \end{bmatrix}$$

    ※ Check eigenvector is unit vector!

Example: PCA

- Find principal components of given data

x	2.5	0.5	2.2	1.9	3.1	2.3	2.0	1.0	1.5	1.1
y	2.4	0.7	2.9	2.2	3.0	2.7	1.6	1.1	1.6	0.9

  - Step 4) Choosing components and forming a loading matrix
    - If you choose two principal components both

$$\mathbf{W} = \begin{bmatrix} -0.678 & -0.735 \\ -0.735 & 0.678 \end{bmatrix}$$

    - If you want to reduce dimensionality

$$\mathbf{W} = \begin{bmatrix} -0.678 \\ -0.735 \end{bmatrix}$$

  - Step 5) Derive the new data set

$$\mathbf{T} = \mathbf{XW}$$

x'	-0.83	1.78	-0.99	-0.27	-1.68	-0.91	0.99	1.14	0.44	1.22
y'	-0.18	0.14	0.38	0.13	-0.21	0.18	-0.35	0.46	0.02	-0.16

Feature Scaling

- PCA finds principal component to achieve the highest variance
  - The variable with large scale is dominated on principal component
    ex) When distance measure is change from m to cm, variance increases $10000(100^2)$ times

Length(m)	Length(cm)
1.5	150
1.7	170
2.3	230
3.3	330
2.7	270
1.9	190

Sample variance(m)=0.46

Sample variance(cm)=4586

- Before apply PCA to data samples, standardization is applied
  - Transform each dimension to have unit variance

Reconstruct to Original Space

- Transformed data by PCA can be reconstructed to original space
  - Recall the final transformation

$$\mathbf{T} = \mathbf{XW}$$

  - Old data can be written as

$$\mathbf{X} = \mathbf{TW}^{-1}$$

    - If $\mathbf{W}$ consists of unit vectors which are orthogonal to each other, inverse matrix of $\mathbf{W}$ is the same as the transpose of $\mathbf{W}$, $\mathbf{W}^T$

$$\therefore \mathbf{X} = \mathbf{TW}^T$$

    - If you substract mean of each dimension from original data

$$\mathbf{X} = \mathbf{TW}^T + \boldsymbol{\mu}$$

      - $\boldsymbol{\mu}$ is mean vector of $\mathbf{X}$ ($\boldsymbol{\mu} = \left[\bar{x}_1 \bar{x}_2 \cdots \bar{x}_p\right]^T$)
    - Actually, if $\mathbf{W}$ is not square matrix(if you choose the smaller number of principal components than original dimension), $\mathbf{W}^{-1}$ does not exist. However, in this case, reconstruction is performed through $\mathbf{W}^T$

Programming Exercise

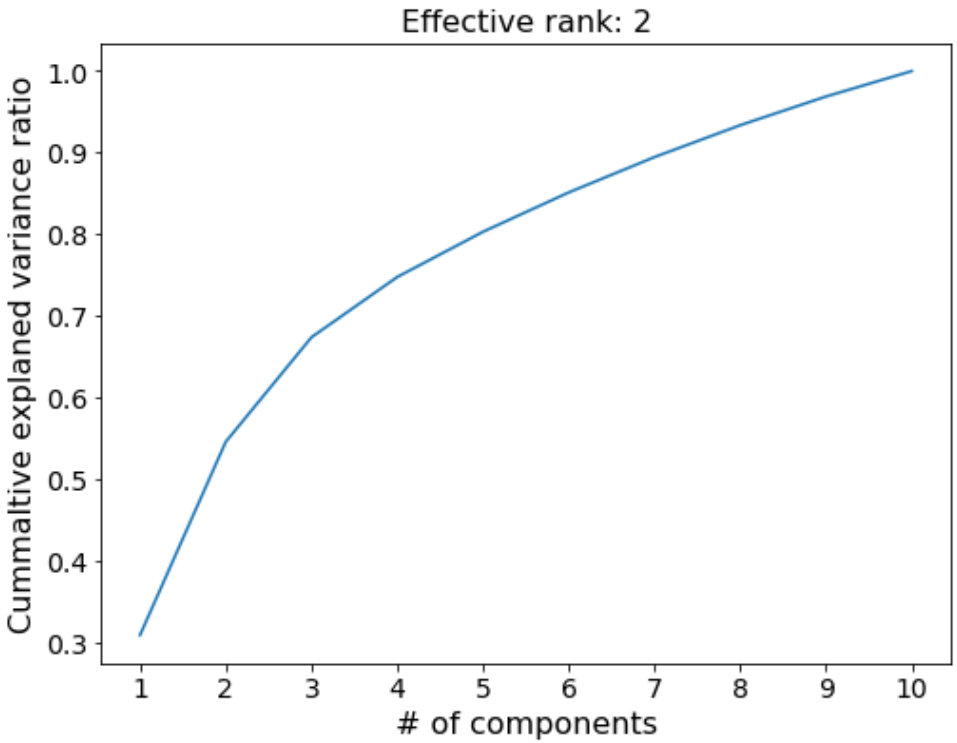
PCA

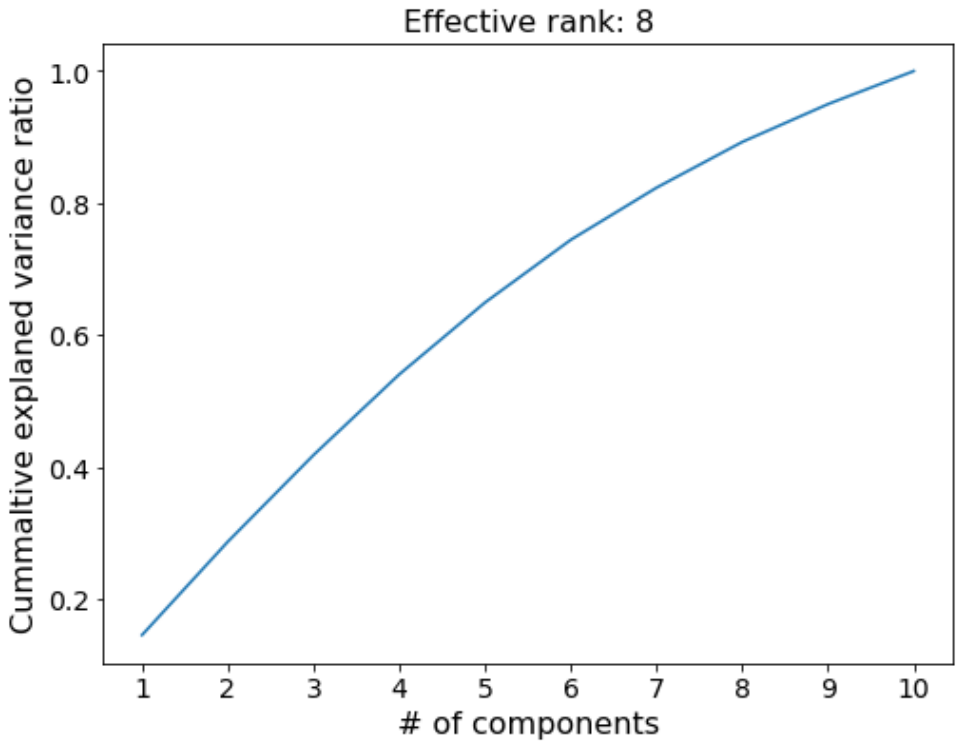
- PCA is implemented by scikit-learn
  - For PCA, use **sklearn.decomposition.PCA**

- Parameters of PCA
  - n_components: number of components to keep
    - If n_components is not set all components are kept (n_components=min(n_samples, n_features))

PCA

- Generate regression data
  - # of features: 10
  - # of informative features: 3
  - effective rank: 2 or 8



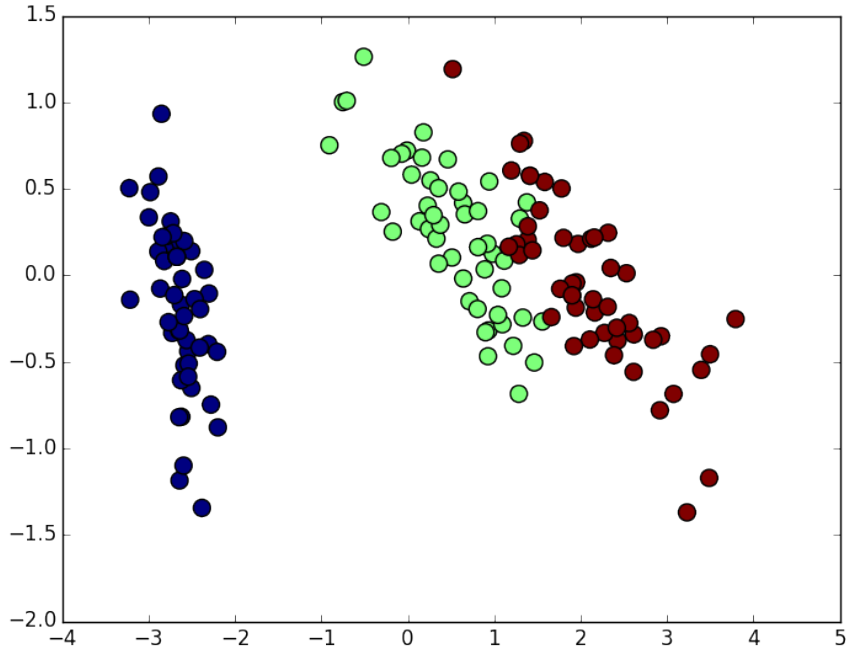


PCA

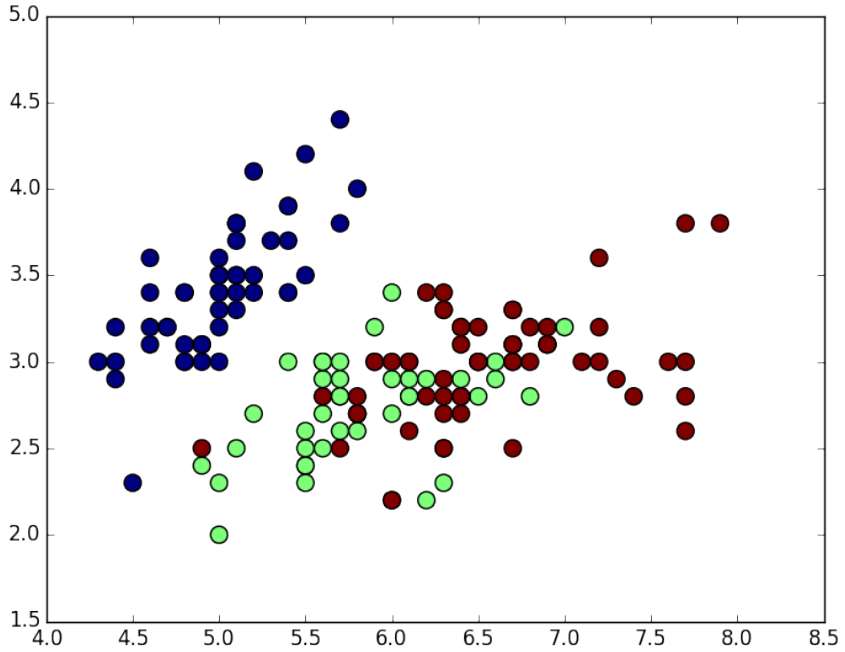
- After finding components, it is possible to project original data samples on components using **transform(*X*)**

```
x_pca=pca.transform(x)
```

  - Compare scatter plots for iris data



x:1st PC y:2nd PC

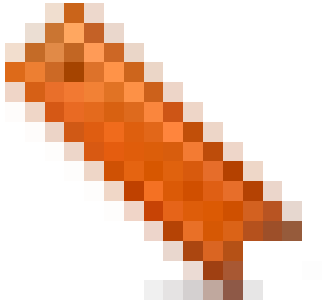


x:1st input y:2nd input

Application: PCA

- Extract important features through PCA for face recognition
  - For image recognition, simple way to represent each image is to vectorization

16×16 image



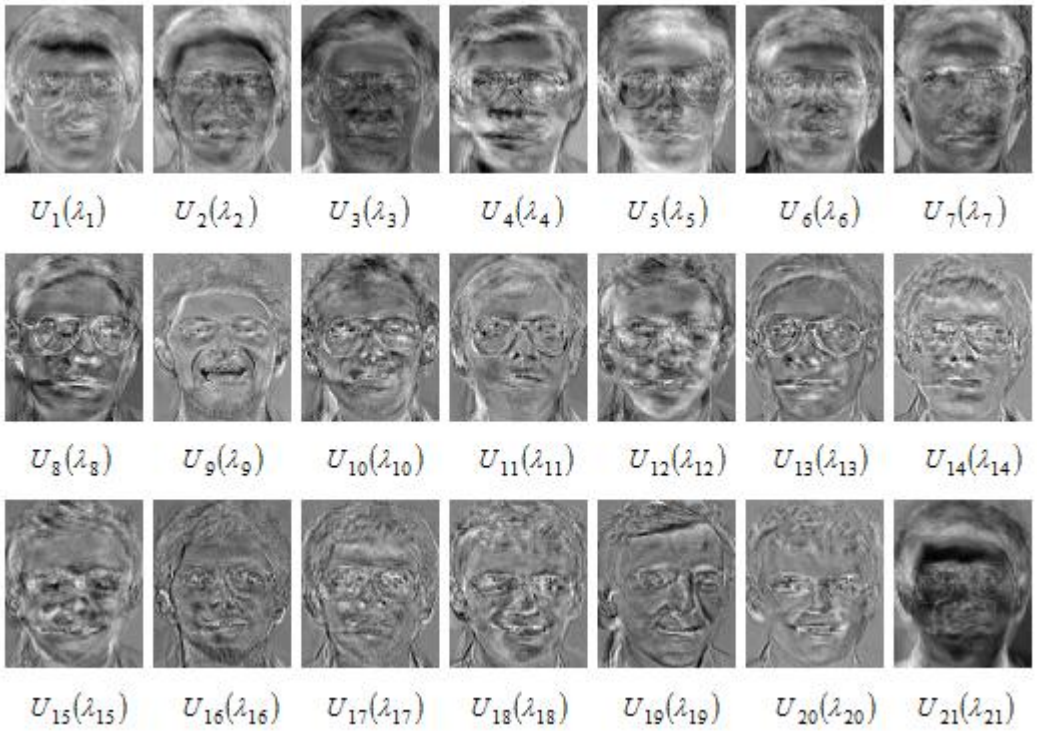
Each pixel represents one dimension

Transform to vector with 256 dimensions

  - Apply PCA to the set of image vectors and obtain principal components → transform image vector to lower dimensional space by loading matrix
    - Usually image is high-dimensional data
    - Through PCA, image can be compressed to low-dimensional data

Application: PCA

- Eigenfaces
  - A set of eigenvectors when they are used in the computer vision problem of human face recognition



  - Eigenface can be viewed as a sort of map of the variations between faces
  - PCA analysis has identified the statistical patterns in the data

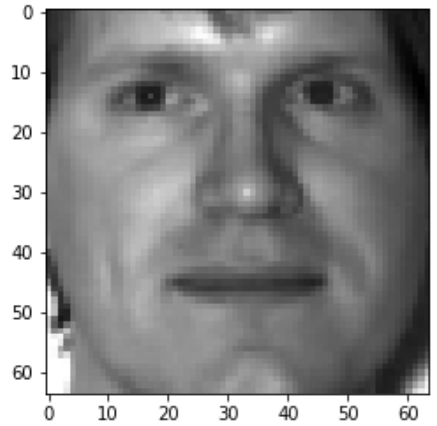
Eigenfaces

- Load Yale database
  - Contains 165 grayscale images from 15 individuals

```
from scipy.io import loadmat
imgs=loadmat(os.path.join(datapath,'Yale_64x64.mat'))
```

    - fea: face images
    - gnd: the label

```
plt.imshow(np.reshape(imgs['fea'][0], (64,64)).T, cmap=plt.cm.gray)
```



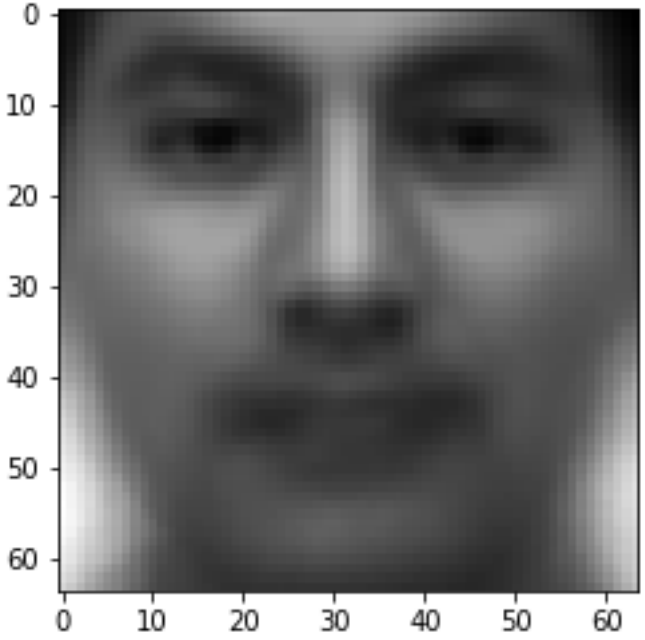
Eigenfaces

- Apply PCA to Yale database
  - Get 10 principal components

- Draw the average face of 165 images and the principal components

Eigenfaces

- The average face



Eigenfaces

- Eigenfaces

Eigenfaces: Classification

- Data partition
  - Yale database contains 165 grayscale images from 15 individuals
    - 11 images for each individual
    - Randomly select one image for each individual → Validation set
    - The remaining images → Training set
  - Build several logistic classifiers
    - Using the original images
    - Using the transformed images
      - # of PCs: from 1 to 150
      - **The loading matrix should be obtained using the training set**
  - Compare the classifiers
    - Accuracy

Eigenfaces: Classification

- Data partition
  - Yale database contains 165 grayscale images from 15 individuals
    - 11 images for each individual
    - Randomly select one image for each individual → Validation set
    - The remaining images → Training set

Eigenfaces: Classification

- Classification results