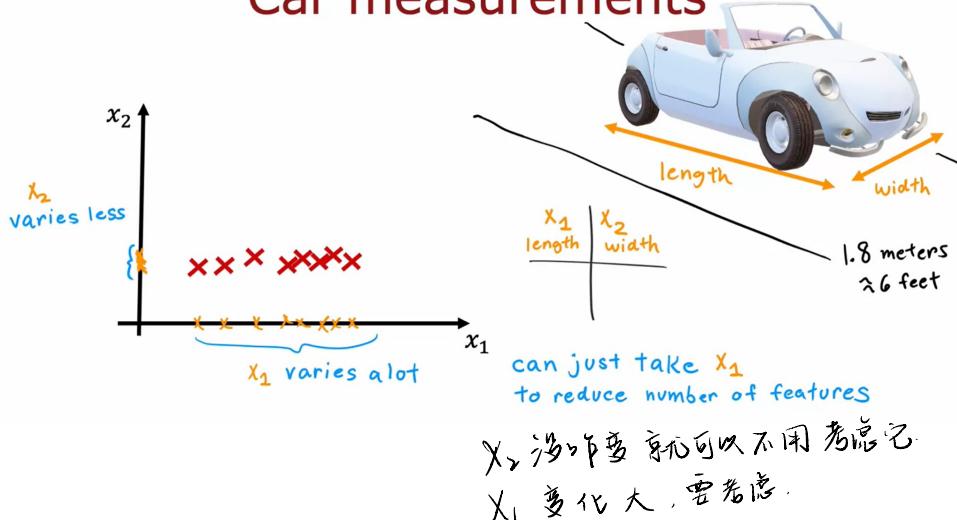


Reducing the number of features.

例題 1:

Car measurements

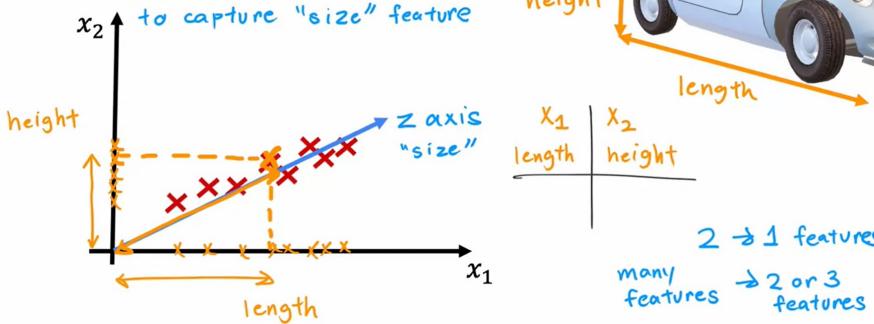


例題 2:

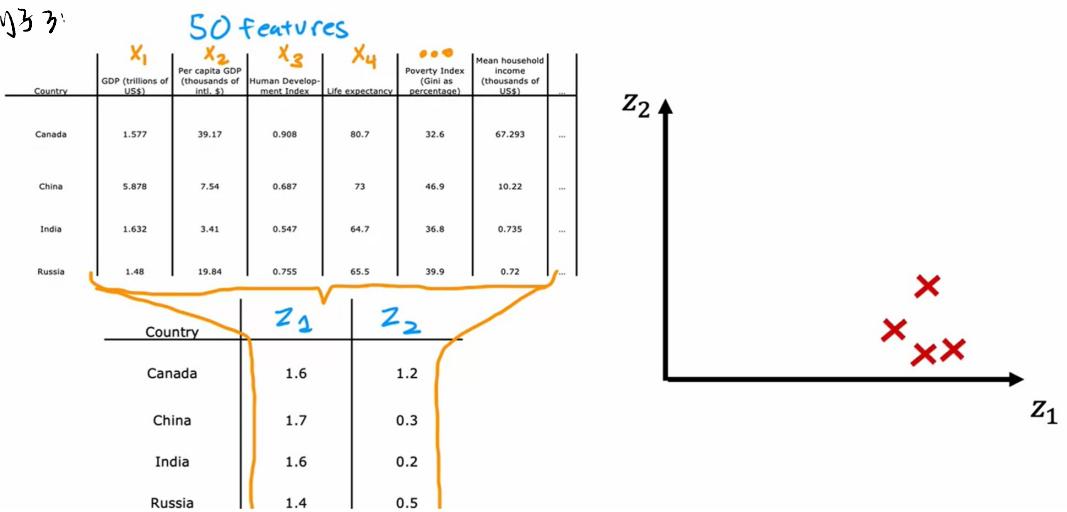
Size

PCA: find new axis and coordinates

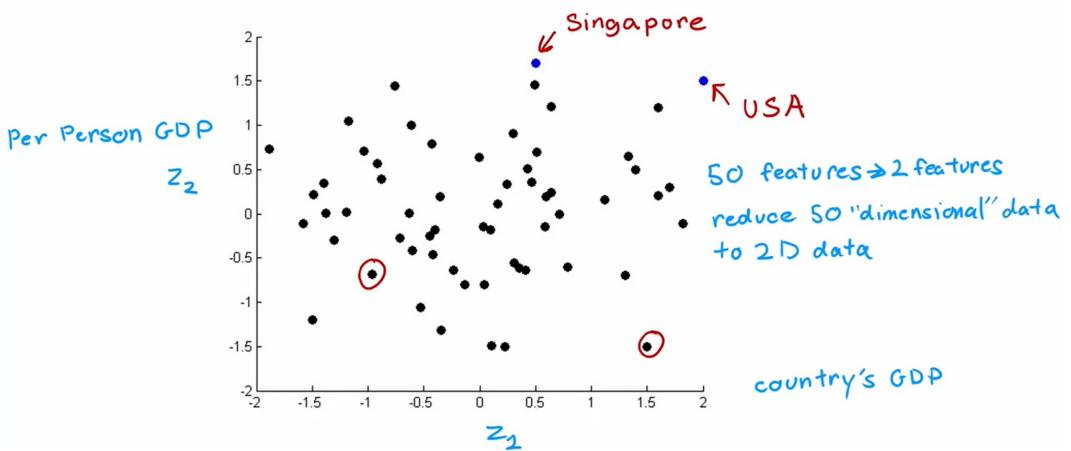
use fewer numbers
to capture "size" feature



17/133:

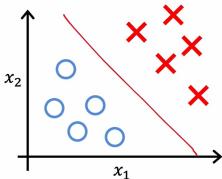


Data visualization



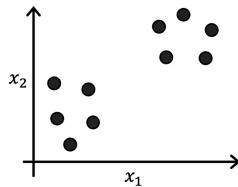
PCA algorithm

Supervised learning



Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), (x^{(3)}, y^{(3)}), \dots, (x^{(m)}, y^{(m)})\}$?

Unsupervised learning



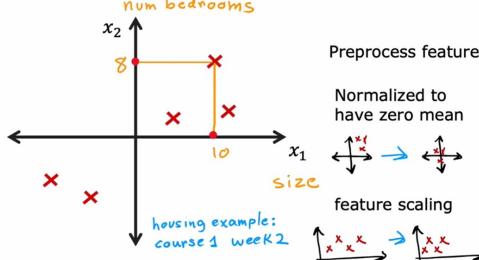
Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \dots, x^{(m)}\}$

沒有 target label y .

PCA algorithm

coordinates
 $x_1 = 10 \quad x_2 = 8$

Can we choose
a different axis?

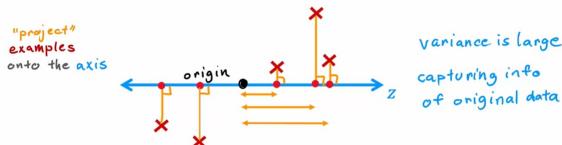


Preprocess features

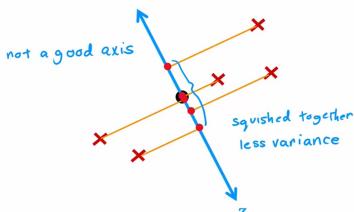
Normalized to
have zero mean

feature scaling

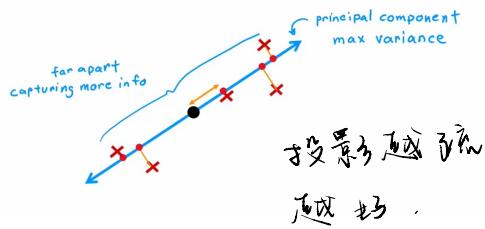
Choose an axis



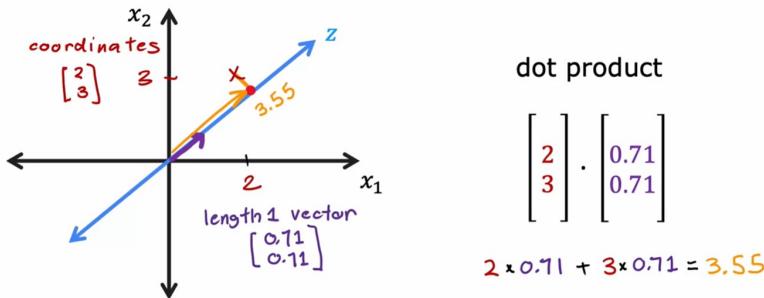
Choose an axis



Choose an axis



Coordinate on the new axis

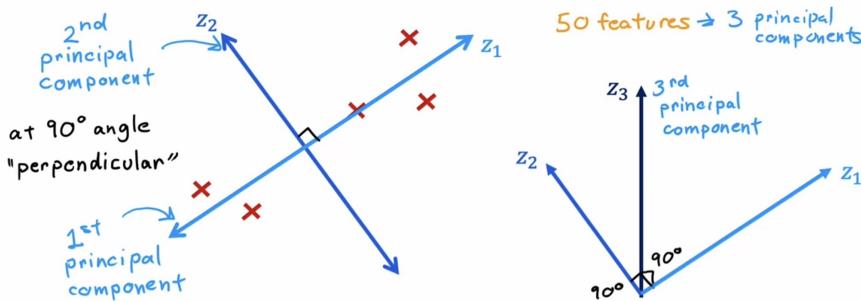


dot product

$$\begin{bmatrix} 2 \\ 3 \end{bmatrix} \cdot \begin{bmatrix} 0.71 \\ 0.71 \end{bmatrix}$$

$$2 \times 0.71 + 3 \times 0.71 = 3.55$$

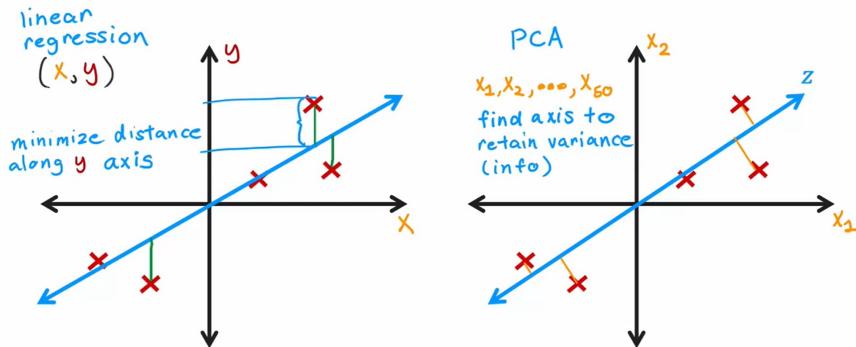
More principal components



如果有 3 个轴

3 个轴相互垂直

PCA is not linear regression



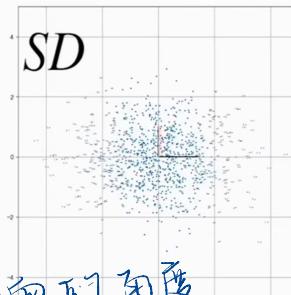
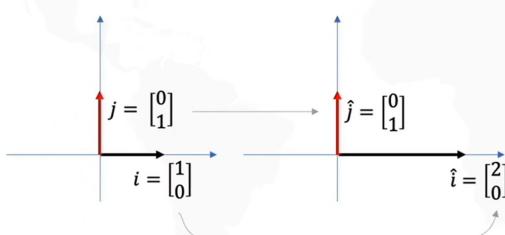
数据线性变换

拉伸

$$D = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \end{bmatrix}$$

只在对角线上有数字

$$S = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \quad SD = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \end{bmatrix} = \begin{bmatrix} 2x_1 & 2x_2 & 2x_3 & 2x_4 \\ y_1 & y_2 & y_3 & y_4 \end{bmatrix}$$



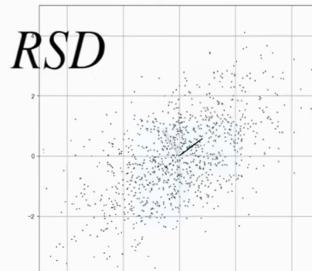
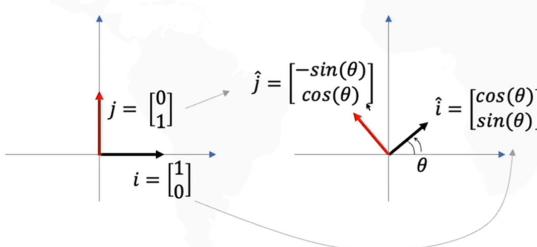
旋转决定了方差最大方向的角度

旋转

$$D = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \end{bmatrix}$$

$$R = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

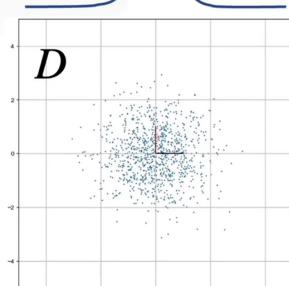
$$RD = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \end{bmatrix}$$



白数据

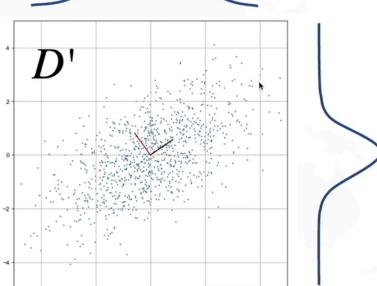
白数据 (white data)

x和y都是标准正态分布
而且x和y不相关



我们手上的数据(去中心化后)

x和y是正态分布但不是标准
x和y相关



白数据

$$S = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \quad R = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

D

白数据 (white data)

$$S^{-1}R^{-1}D'$$

拉伸

$$R^{-1}D'$$

旋转

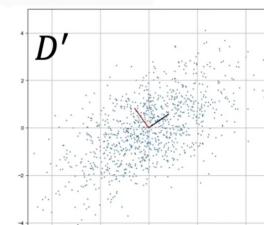
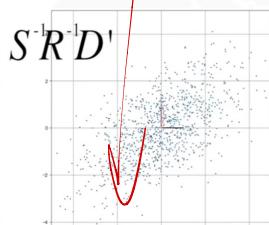
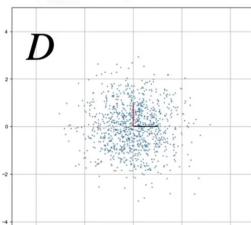
$$D'$$

我们手上的数据

$$D = S^{-1}R^{-1}D'$$

$$S^{-1} = \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix}$$

$$R^{-1} = \begin{bmatrix} \cos(-\theta) & -\sin(-\theta) \\ \sin(-\theta) & \cos(-\theta) \end{bmatrix} = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} = R^T$$



协方差的特征向量就是 R

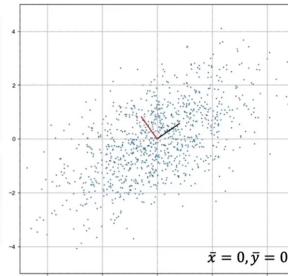
协方差:

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

协方差表示的是:

两个变量在变化过程中是同方向变化? 还是反方向变化? 同向或反向程度如何?

$$x \uparrow \rightarrow y \uparrow \rightarrow \text{cov}(x, y) > 0$$



$$\text{cov}(x, y) = \frac{\sum_{i=1}^n x_i y_i}{n-1} \quad \text{cov}(x, x) = \frac{\sum_{i=1}^n x_i^2}{n-1}$$

方差

协方差矩阵:

$$C = \begin{bmatrix} \text{cov}(x, x) & \text{cov}(x, y) \\ \text{cov}(y, x) & \text{cov}(y, y) \end{bmatrix} \quad \begin{array}{l} \text{对称阵} \\ \text{对角线是方差} \end{array}$$

协方差矩阵:

对称阵
对角线是方差

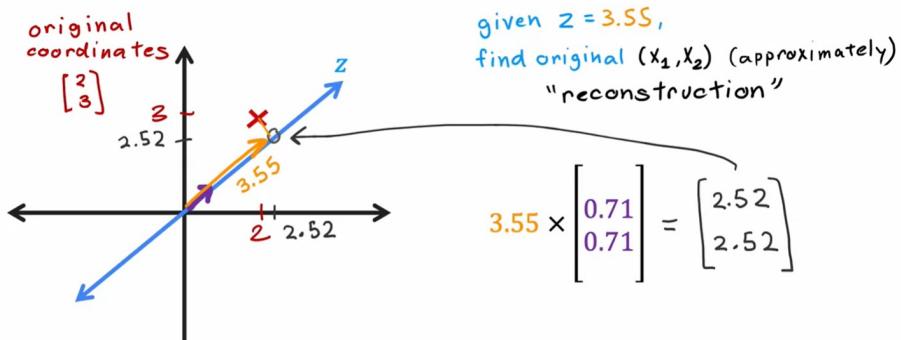
$$C = \begin{bmatrix} \frac{\sum_{i=1}^n x_i^2}{n-1} & \frac{\sum_{i=1}^n x_i y_i}{n-1} \\ \frac{\sum_{i=1}^n x_i y_i}{n-1} & \frac{\sum_{i=1}^n y_i^2}{n-1} \end{bmatrix} \quad \begin{array}{l} \text{cov}(x, y) = \frac{\sum_{i=1}^n x_i y_i}{n-1} \\ \text{cov}(x, x) = \frac{\sum_{i=1}^n x_i^2}{n-1} \end{array}$$

$$= \frac{1}{n-1} \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \end{bmatrix} \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \\ x_4 & y_4 \end{bmatrix}$$

$$= \frac{1}{n-1} DD^T \quad D - \text{数据}$$

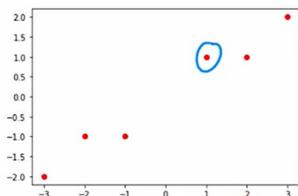
Reconstruction

Approximation to the original data



PCA in code.

1D

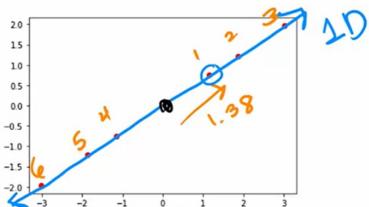


Example

```
X = np.array([[1, 1], [2, 1], [3, 2],
[-1, -1], [-2, -1], [-3, -2]])
```

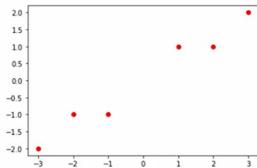
2D

```
pca_1 = PCA(n_components=1)
pca_1.fit(X)
pca_1.explained_variance_ratio_ 0.992
X_trans_1 = pca_1.transform(X)
X_reduced_1 = pca_1.inverse_transform(X_trans_1)
```



```
array([
1 [ 1.38340578], ←
2 [ 2.22189802], ←
3 [ 3.6053038 ],
4 [-1.38340578],
5 [-2.22189802],
6 [-3.6053038 ]])
```

27.

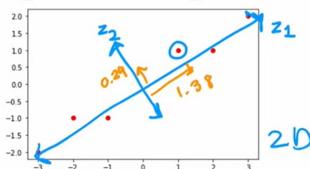


Example

```
X = np.array([[1, 1], [2, 1], [3, 2],  
[-1, -1], [-2, -1], [-3, -2]])
```

2D

```
pca_2 = PCA(n_components=2)  
pca_2.fit(X)  
pca_2.explained_variance_ratio_  $z_1 \quad z_2$   
X_trans_2 = pca.transform(X)  $0.912 \quad 0.008$   
X_reduced_2 = pca.inverse_transform(X_trans_2)
```



z_1 z_2
array([
→[1.38340578, 0.2935787],
[2.22189802, -0.25133484],
[3.6053038 , 0.04224385],
[-1.38340578, -0.2935787],
[-2.22189802, 0.25133484],
[-3.6053038 , -0.04224385]])

2D