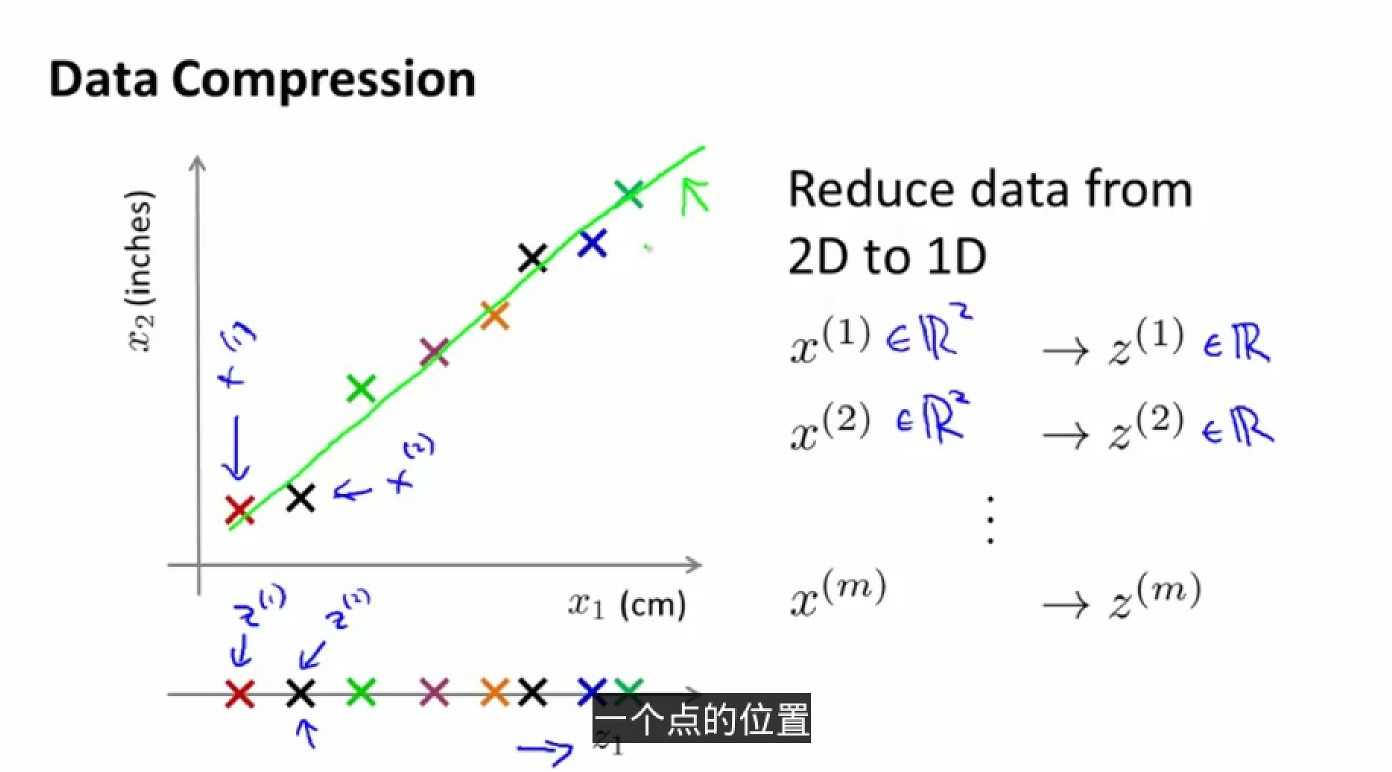
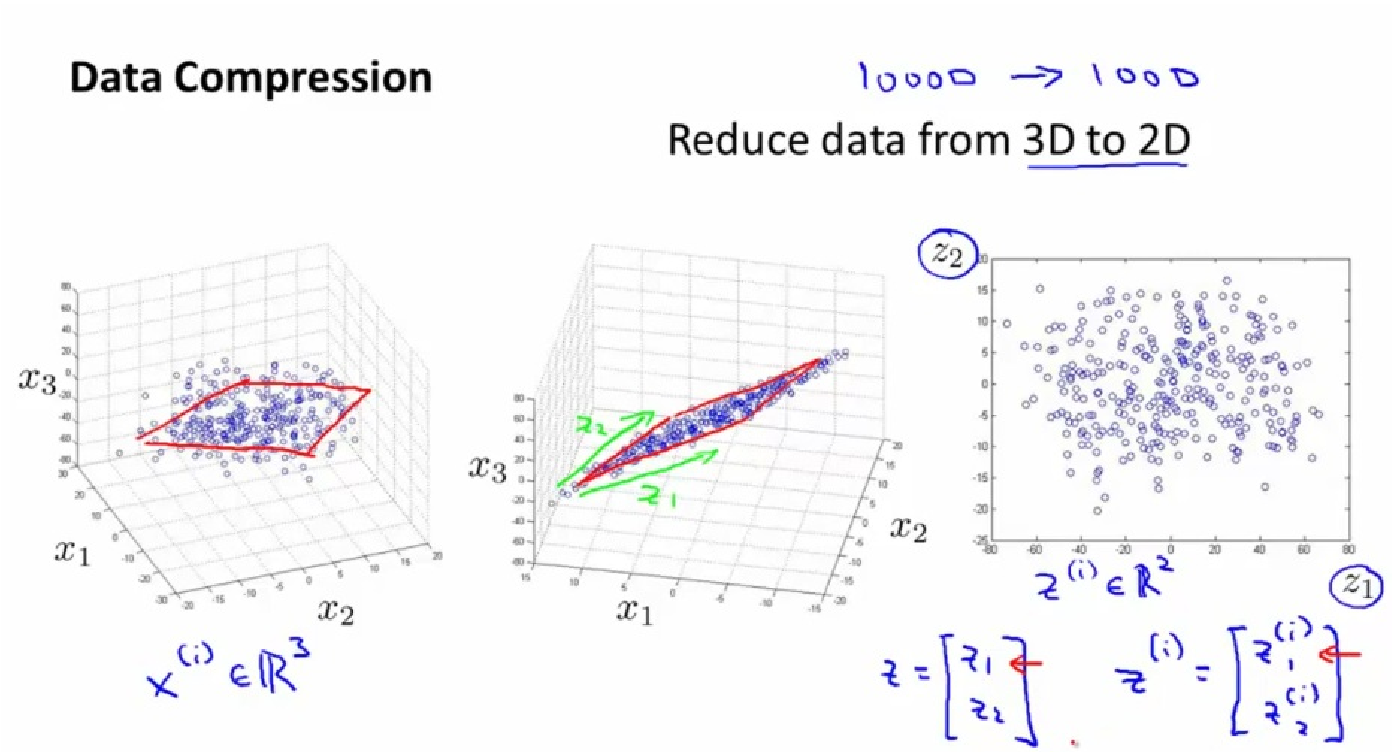
1. 维数约简（dimensionality reduction）-数据压缩 Data Compression

2D降低到1D：



3D降低到2D：



第二个应用=>可视化数据（Data Visualization）

Data Visualization

$x \in \mathbb{R}^{50}$ $x^{(i)} \in \mathbb{R}^{50}$

Country	x_1 GDP (trillions of US$)	x_2 Per capita GDP (thousands of intl. $)	x_3 Human Develop-ment Index	x_4 Life expectancy	x_5 Poverty Index (Gini as percentage)	x_6 Mean household income (thousands of US$)	…
Canada	1.577	39.17	0.908	80.7	32.6	67.293	…
China	5.878	7.54	0.687	73	46.9	10.22	…
India	1.632	3.41	0.547	64.7	36.8	0.735	…
Russia	1.48	19.84	0.755	65.5	39.9	0.72	…
Singapore	0.223	56.69	0.866	80	42.5	67.1	…
USA	14.527	46.86	0.91	78.3	40.8	84.3	…
…	…	…	…	…	…	…	

resources from en.wikipedia.org]

Andrew Ng

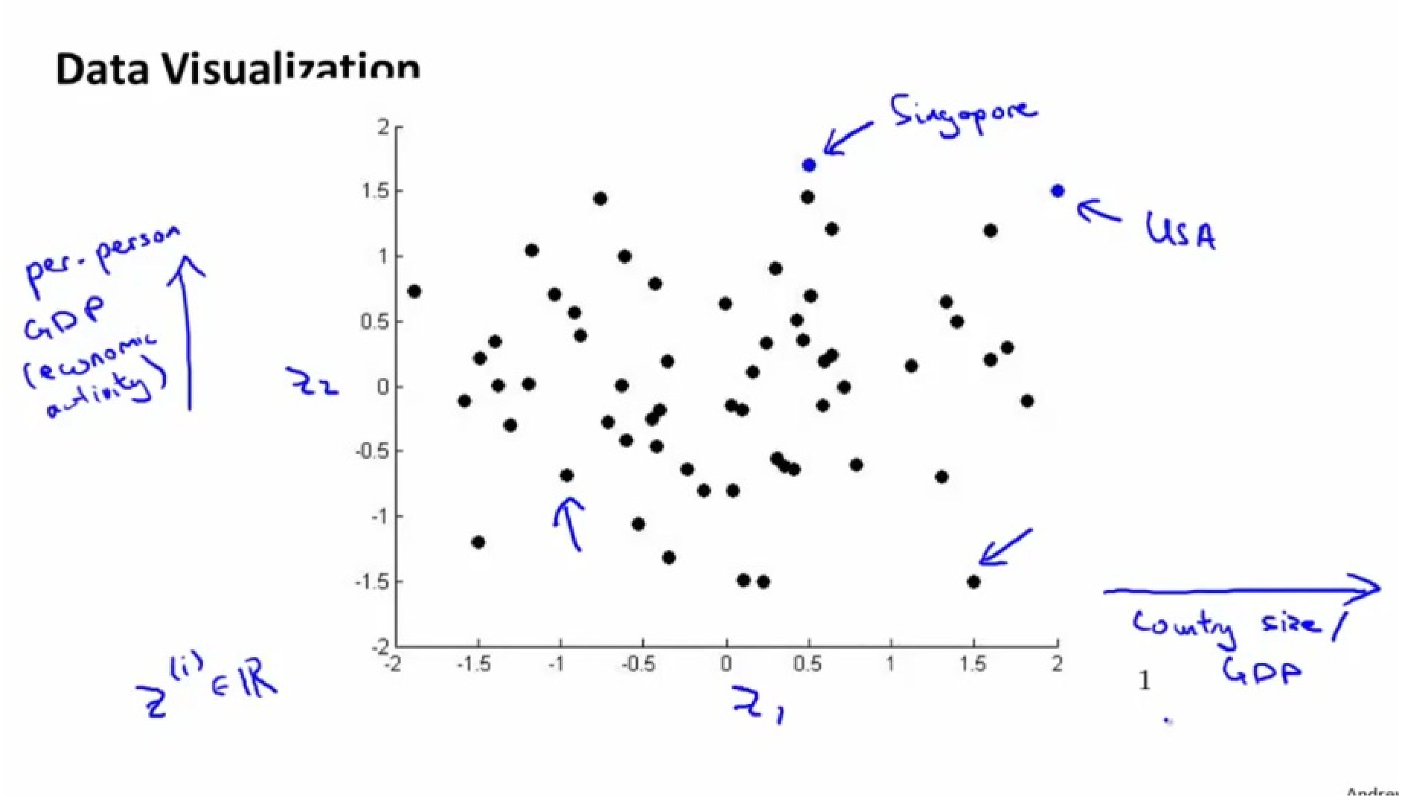
Data Visualization

$z^{(i)} \in \mathbb{R}^2$

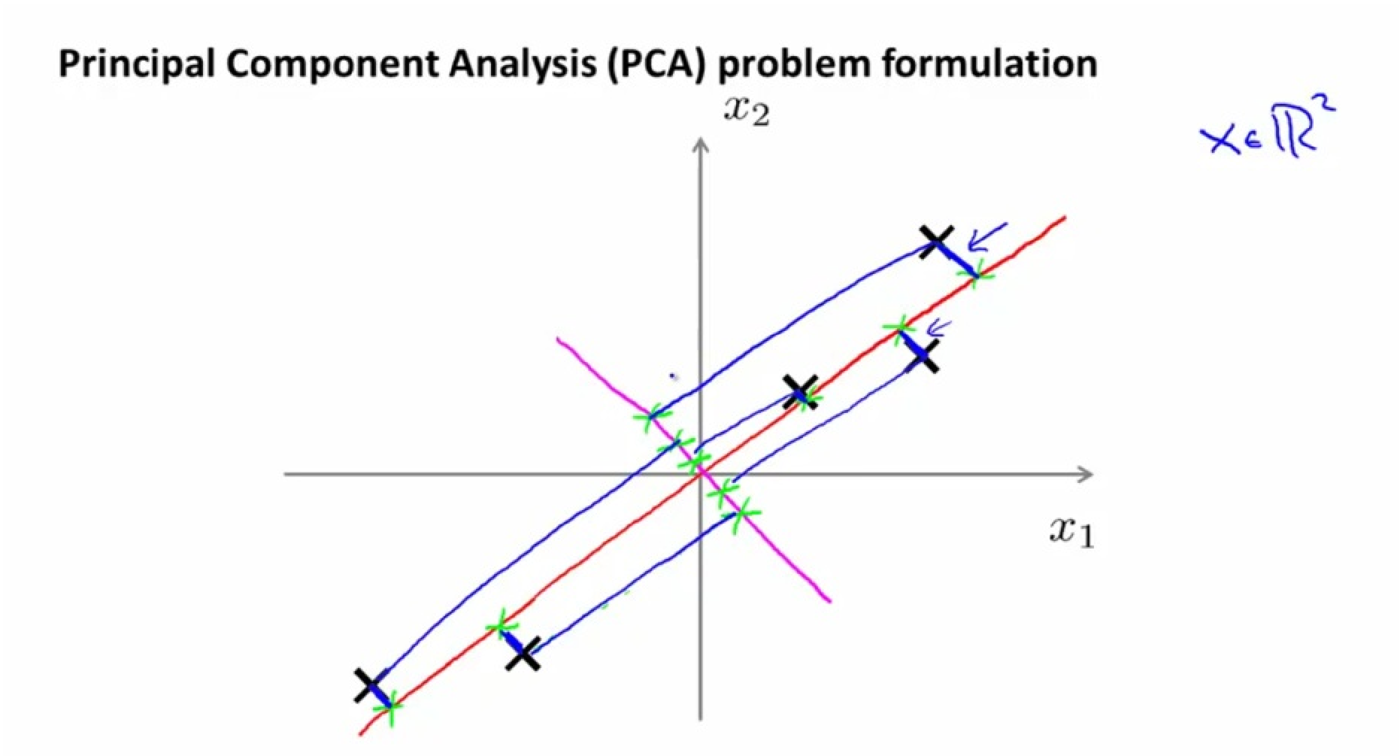
Country	z_1	z_2
Canada	1.6	1.2
China	1.7	0.3
India	1.6	0.2
Russia	1.4	0.5
Singapore	0.5	1.7
USA	2	1.5
…	…	…

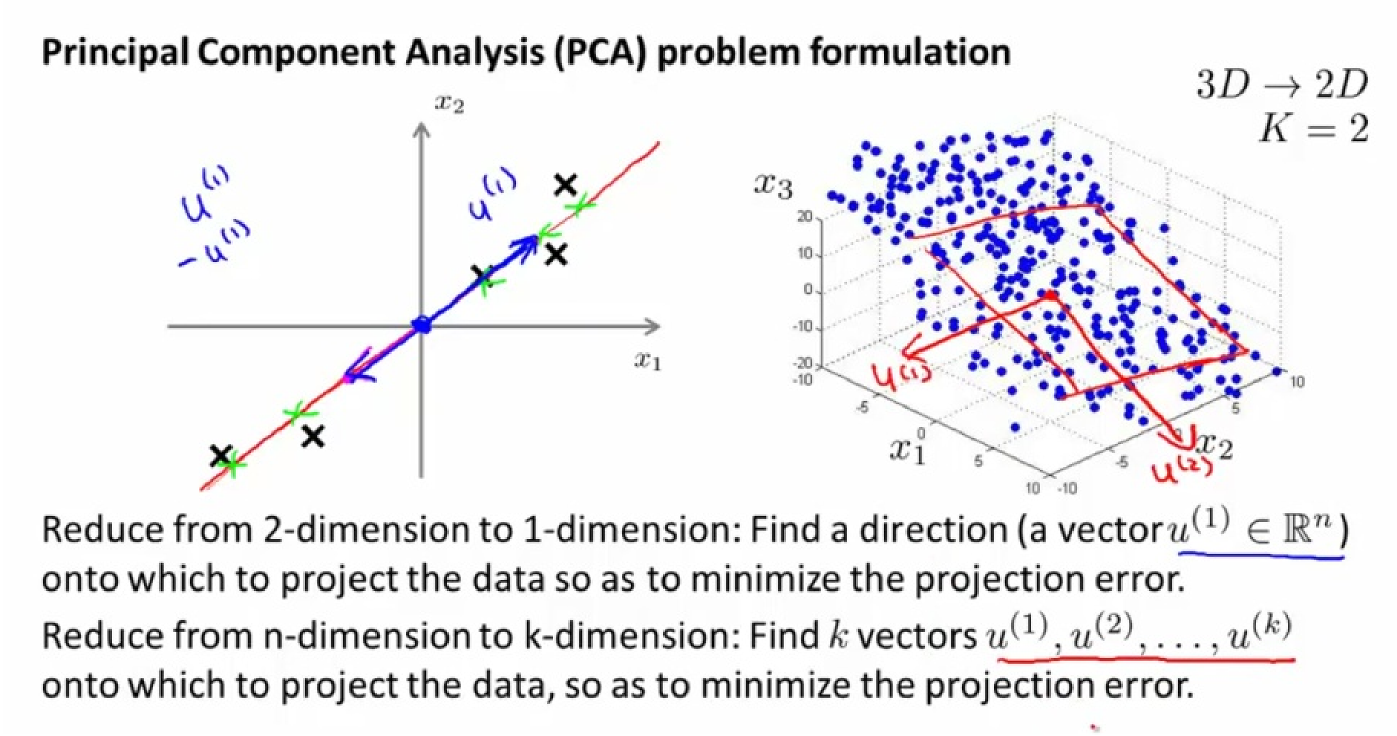
Reduce data from 50D to 2D

你想要的这些二维新特征一个物理含义

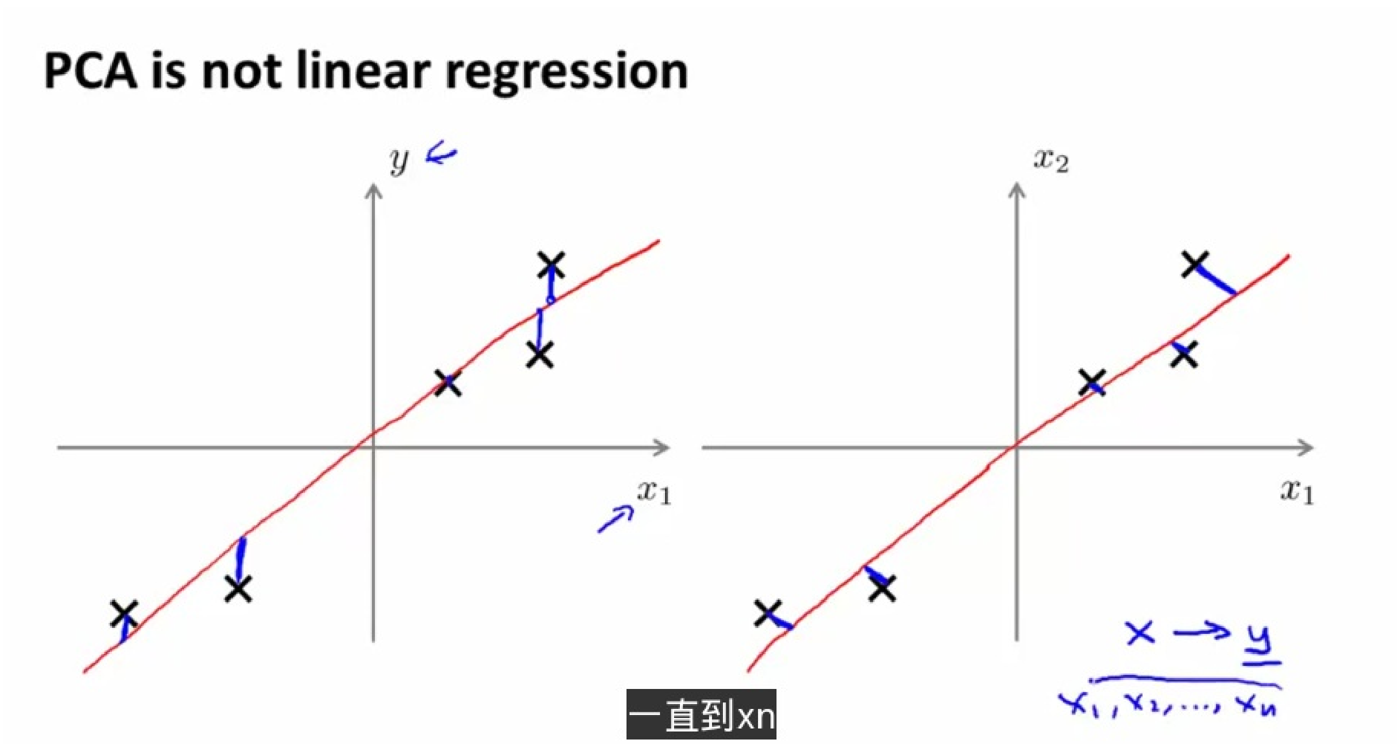


2. 主成分分析（PCA，Principal Component Analysis）：寻找一个低维平面使得点投影到其上投影误差最小。





PCA和线性回归比较：



使用PCA算法：

（1）均值标准化和特征缩放；

Data preprocessing

Training set: $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$ ←

Preprocessing (feature scaling/mean normalization):

$$\mu_j = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)}$$

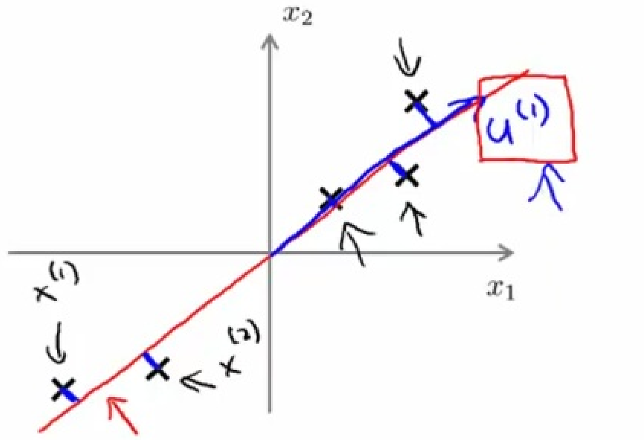
Replace each $x_j^{(i)}$ with $x_j - \mu_j$.

If different features on different scales (e.g., $x_1 =$ size of house, $x_2 =$ number of bedrooms), scale features to have comparable range of values.

$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j}$$

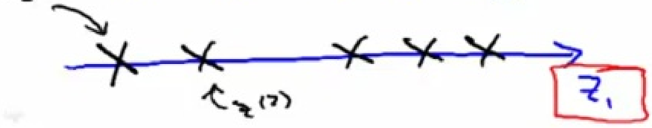
接下来就正式进入 PCA 的算法部分

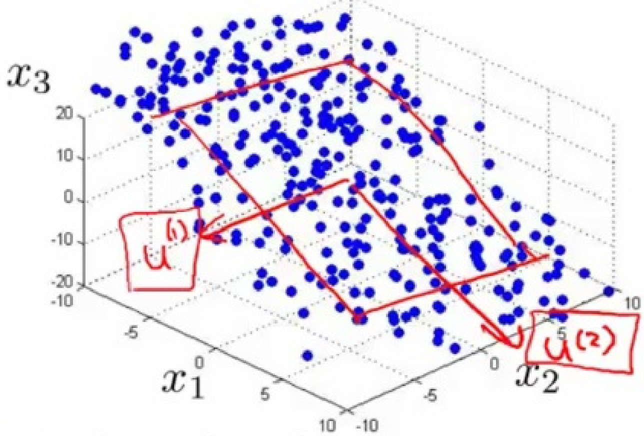
Principal Component Analysis (PCA) algorithm



Reduce data from 2D to 1D

$x^{(i)} \in \mathbb{R}^2 \rightarrow z^{(i)} \in \mathbb{R}$





Reduce data from 3D to 2D

$x^{(i)} \in \mathbb{R}^3 \rightarrow z^{(i)} \in \mathbb{R}^2$

$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

Andrew

Principal Component Analysis (PCA) algorithm

Reduce data from n-dimensions to k-dimensions

Compute "covariance matrix":

$$\Sigma = \frac{1}{m}\sum_{i=1}^{n} \boxed{\underbrace{(x^{(i)})}_{n\times 1}\underbrace{(x^{(i)})^T}_{1\times n}} \quad n\times n$$

Sigma

Compute "eigenvectors" of matrix Σ:

→ Singular value decomposition

eig (Sigma)

```
[U,S,V] = svd(Sigma);
```

n×n matrix.

$$U = \begin{bmatrix} | & | & | & & | \\ u^{(1)} & u^{(2)} & u^{(3)} & \dots & u^{(m)} \\ | & | & | & & | \end{bmatrix}$$

$U \in \mathbb{R}^{n\times n}$

$u^{(1)}, \dots, u^{(k)}$

k

k 个方向

Principal Component Analysis (PCA) algorithm

From `[U,S,V] = svd(Sigma)`, we get:

$$\rightarrow U = \begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \dots & u^{(n)} \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n\times n}$$

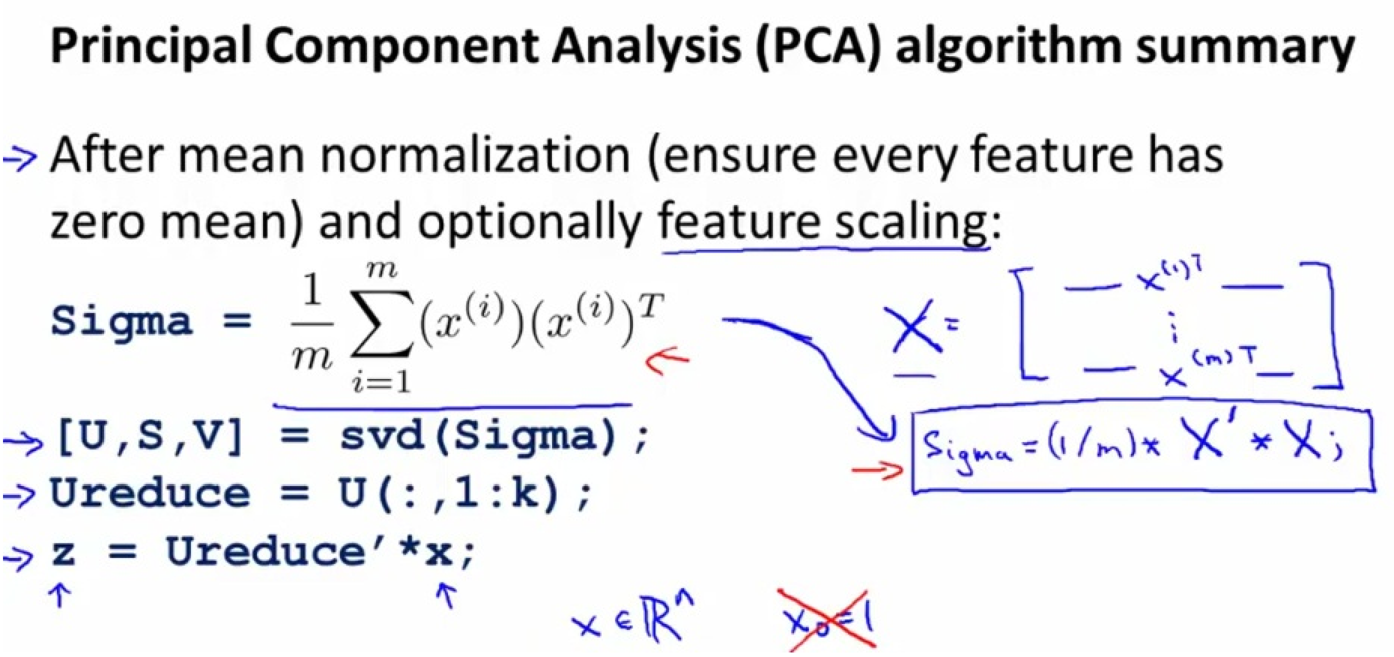
k

$x \in \mathbb{R}^n \rightarrow z \in \mathbb{R}^k$

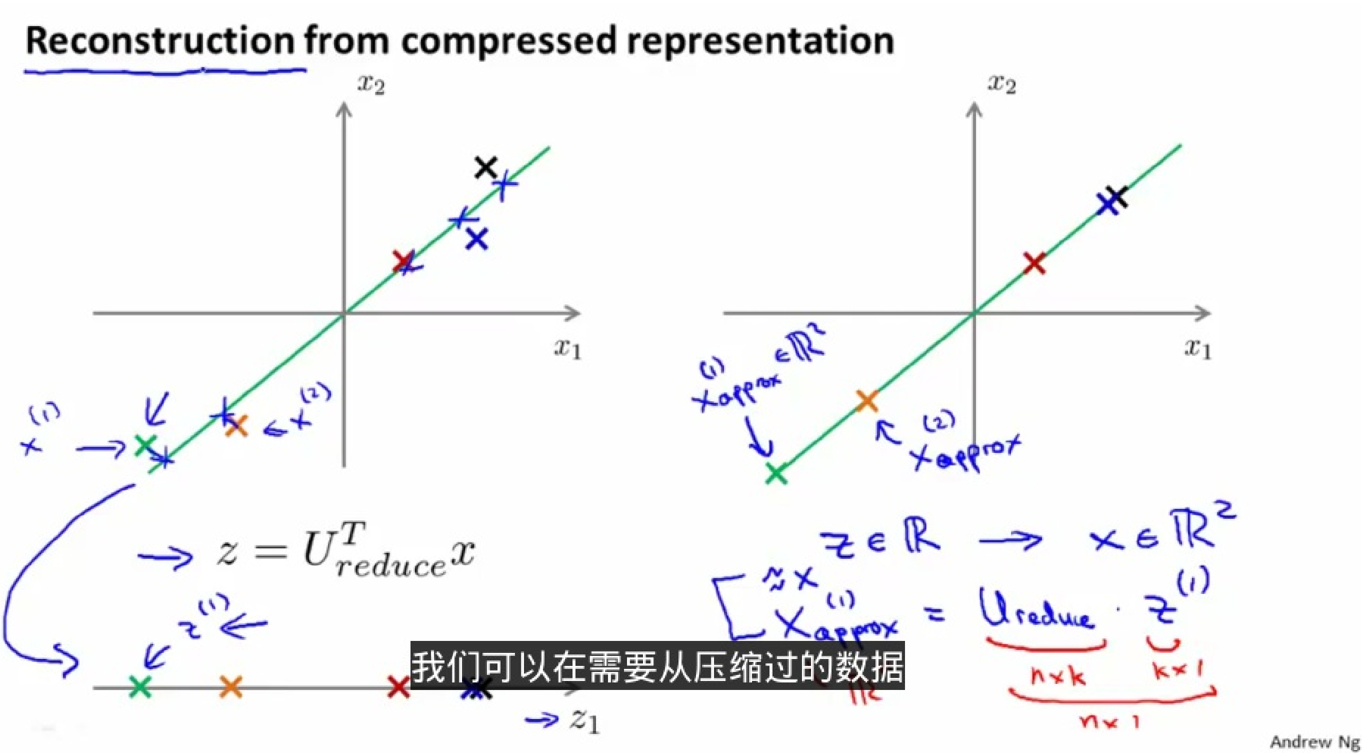
$$z^{(i)} = \underbrace{\begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \dots & u^{(k)} \\ | & | & & | \end{bmatrix}^T}_{U_{reduce}} x^{(i)} = \underbrace{\underbrace{\begin{bmatrix} — (u^{(1)})^T — \\ \vdots \\ — (u^{(k)})^T — \end{bmatrix}}_{k\times n} \underbrace{x^{(i)}}_{n\times 1}}_{k\times 1}$$

$z \in \mathbb{R}^k$

降维得到的就是 z(i)



从压缩后的维重构成高维：



k选择：

Choosing k (number of principal components)

Average squared projection error: $\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x^{(i)}_{approx}\|^2$

Total variation in the data: $\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2$

Typically, choose k to be smallest value so that

$$\frac{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x^{(i)}_{approx}\|^2}{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2} \le \cancel{0.01} \qquad \cancel{(1\%)}$$

$\cancel{0.05}$ $\cancel{5\%}$

0.10 (10%)

"~~99%~~ of variance is retained"

~~95%~~ 90%

为了保留99%的差异性

Choosing k (number of principal components)

Algorithm:

Try PCA with $\cancel{k = 1}$ $\cancel{k=2}$ $\cancel{k=3}$ $k=4$ ...

Compute $U_{reduce}, z^{(1)}, z^{(2)}, \ldots, z^{(m)}, x^{(1)}_{approx}, \ldots, x^{(m)}_{approx}$

Check if

$$\boxed{\frac{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x^{(i)}_{approx}\|^2}{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2}} \le 0.01?$$

$k = 17$

```
[U,S,V] = svd(Sigma)
```

$$S = \begin{bmatrix} S_{11} & & & & 0 \\ & S_{22} & & & \\ & & S_{33} & & \\ & & & \ddots & \\ 0 & & & & S_{nn} \end{bmatrix}$$

$k=3$

For given k

$$1 - \frac{\sum_{i=1}^{k} S_{ii}}{\sum_{i=1}^{n} S_{ii}} \le 0.01$$

$$\frac{\sum_{i=1}^{k} S_{ii}}{\sum_{i=1}^{n} S_{ii}} \ge 0.99$$

Choosing k (number of principal components)

```
[U,S,V] = svd(Sigma)
```

Pick smallest value of k for which

$$\boxed{\frac{\sum_{i=1}^{k} S_{ii}}{\sum_{i=1}^{m} S_{ii}}} \geq 0.99$$

k=100

(99% of variance retained)

3. 使用PCA加速学习算法。

监督学习加速：

Supervised learning speedup

$x^{(i)} \in \mathbb{R}^{10,000}$

100

100

$\boxed{(x^{(1)}, y^{(1)})}, (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$

Extract inputs:

Unlabeled dataset: $x^{(1)}, x^{(2)}, \ldots, x^{(m)} \in \mathbb{R}^{10000}$

$\downarrow PCA$

$x \rightarrow z$

$z^{(1)}, z^{(2)}, \ldots, z^{(m)} \in \mathbb{R}^{1000}$

U_{reduce}

New training set:

$\boxed{(z^{(1)}, y^{(1)})}, (z^{(2)}, y^{(2)}), \ldots, (z^{(m)}, y^{(m)})$

$h_\theta(z) = \frac{1}{1+e^{-\theta^T z}}$

Note: Mapping $x^{(i)} \rightarrow z^{(i)}$ should be defined by running PCA only on the training set. This mapping can be applied as well to the examples $x_{cv}^{(i)}$ and $x_{test}^{(i)}$ 并扩展可以 in the cross validation and test sets.

$x \rightarrow z$

Bad use of PCA: To prevent overfitting

- Use $z^{(i)}$ instead of $x^{(i)}$ to reduce the number of features to $k < n$. — 10000
  Thus, fewer features, less likely to overfit.

1000

Bad!

This might work OK, but isn't a good way to address overfitting. Use regularization instead.

$$\min_\theta \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \boxed{\frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2}$$

我们使用正则化的方法来代替PCA方法

PCA is sometimes used where it shouldn't be

Design of ML system:

- Get training set $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})\}$
- ~~Run PCA to reduce $x^{(i)}$ in dimension to get $z^{(i)}$~~
- Train logistic regression on $\{(\cancel{z^{(1)}}\, x^{(1)}, y^{(1)}), \ldots, (\cancel{z^{(m)}}\, x^{(m)}, y^{(m)})\}$
- Test on test set: Map $x_{test}^{(i)}$ to $z_{test}^{(i)}$. Run $h_\theta(z)$ on $\{(z_{test}^{(1)}, y_{test}^{(1)}), \ldots, (z_{test}^{(m)}, y_{test}^{(m)})\}$

- How about doing the whole thing without using PCA?
- Before implementing PCA, first try running whatever you want to do with the original/raw data $\boxed{x^{(i)}}$. Only if that doesn't do what you want, then implement PCA and consider using $z^{(i)}$.

一开始不要将