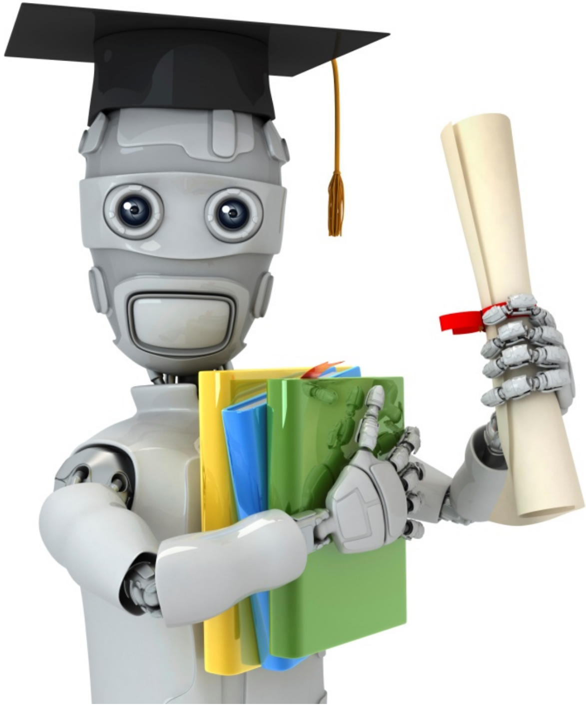
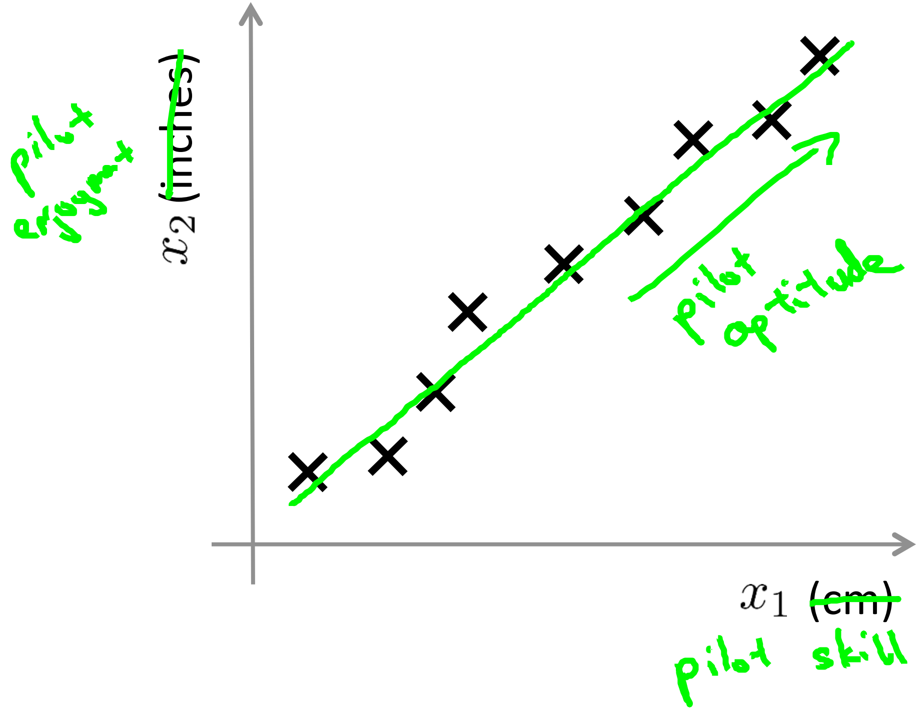


Machine Learning

Dimensionality Reduction

Motivation I: Data Compression

Data Compression



Reduce data from 2D to 1D

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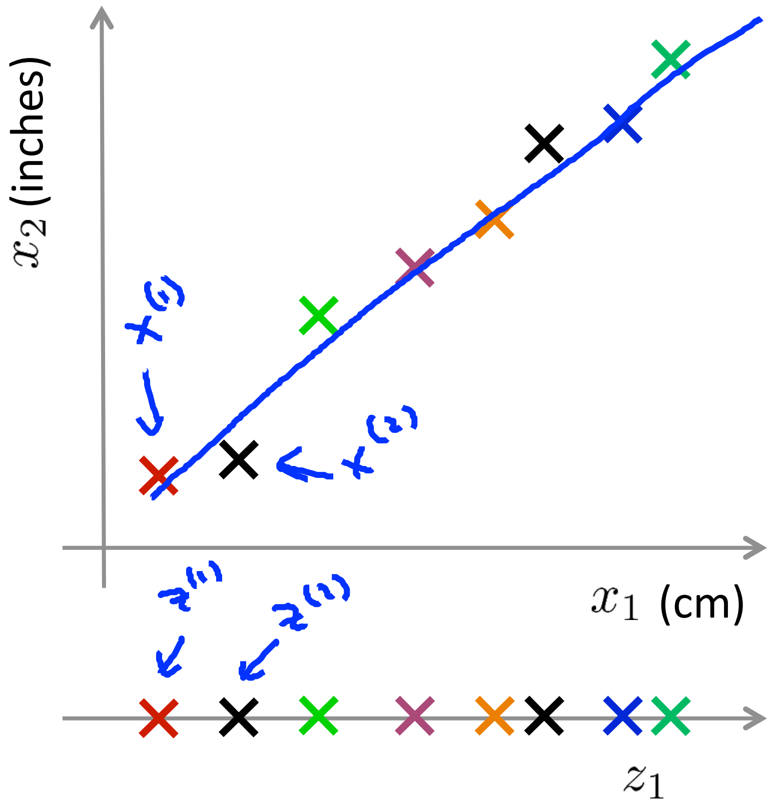
Data Compression



Reduce data from 2D to 1D

$x^{(1)} \in \mathbb{R}^2 \rightarrow z^{(1)} \in \mathbb{R}$

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

$\vdots$

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

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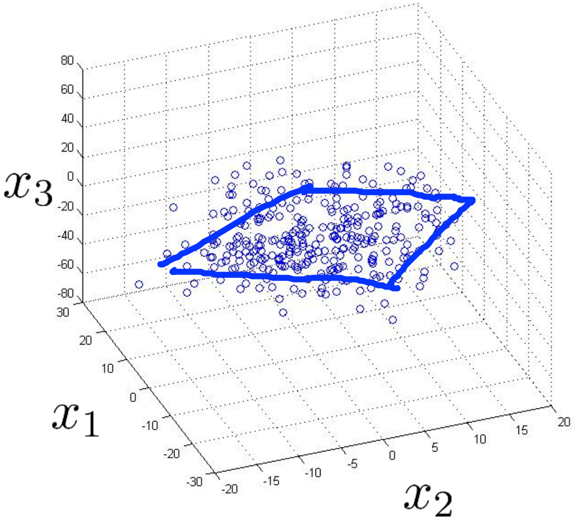
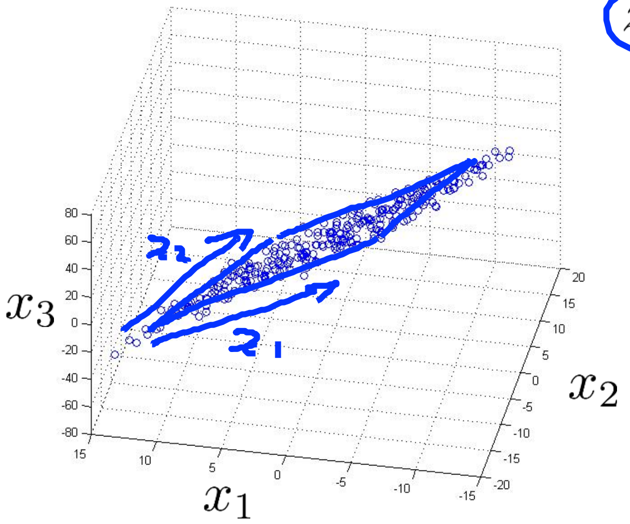
Data Compression

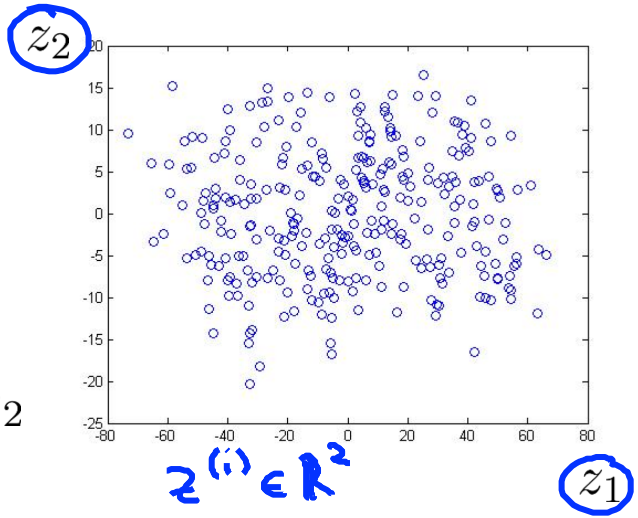
$1000D \rightarrow 100D$

Reduce data from 3D to 2D



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





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

$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$ $\quad z^{(i)} = \begin{bmatrix} z_1^{(i)} \\ z_2^{(i)} \end{bmatrix}$

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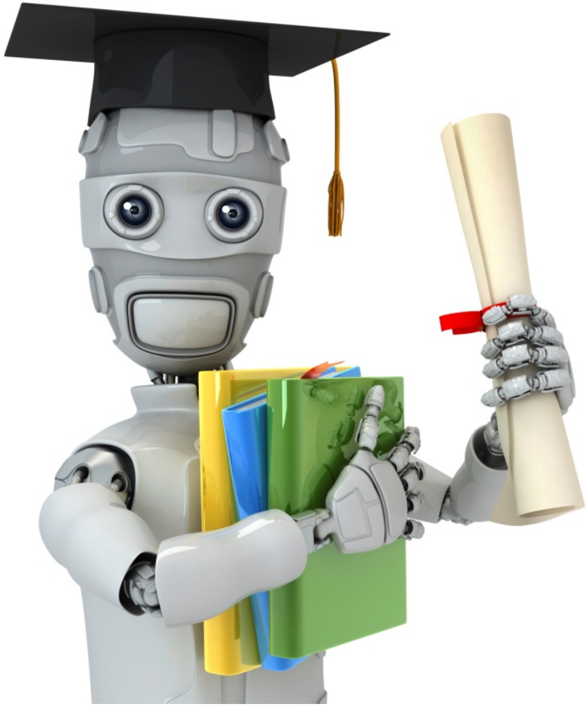


Machine Learning

Dimensionality Reduction

Motivation II: 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]

我们可以使用一对数字 z1和z2 从某种程度来说 这两个数总结了50个数

Data Visualization

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

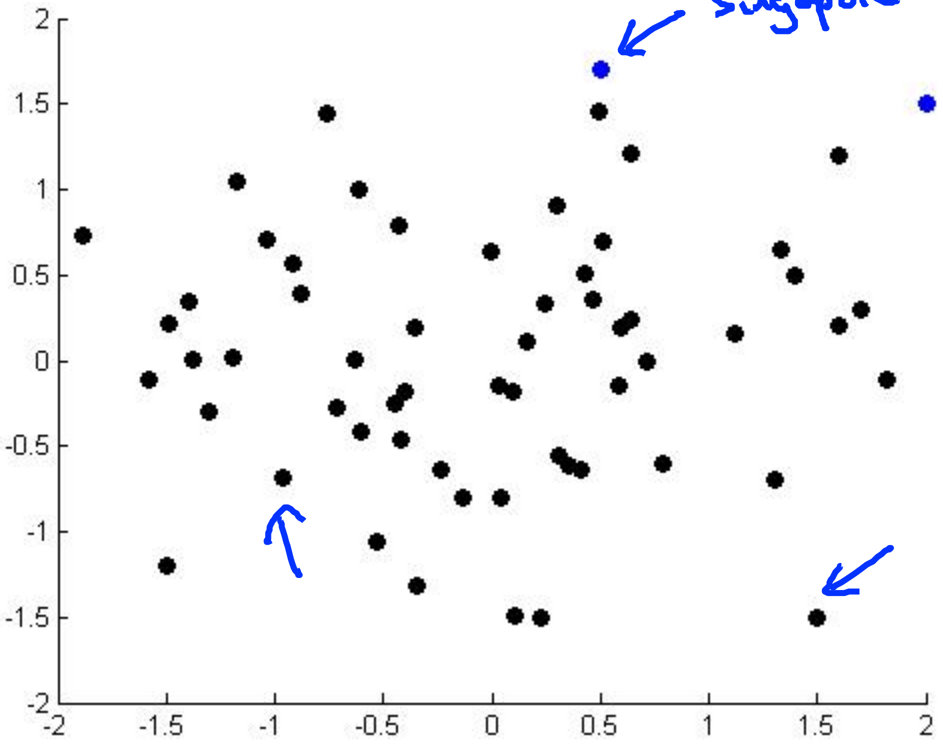
Country	z_1	z_2
Canada	1.6	1.2
China	1.7	0.3
India	1.6	0.2
Russia	1.4	0.5
Singapore	0.5	1.7
USA	2	1.5
…	…	…

Reduce data from 50D to 2D

Data Visualization

per. person GDP (economic activity)

z_2

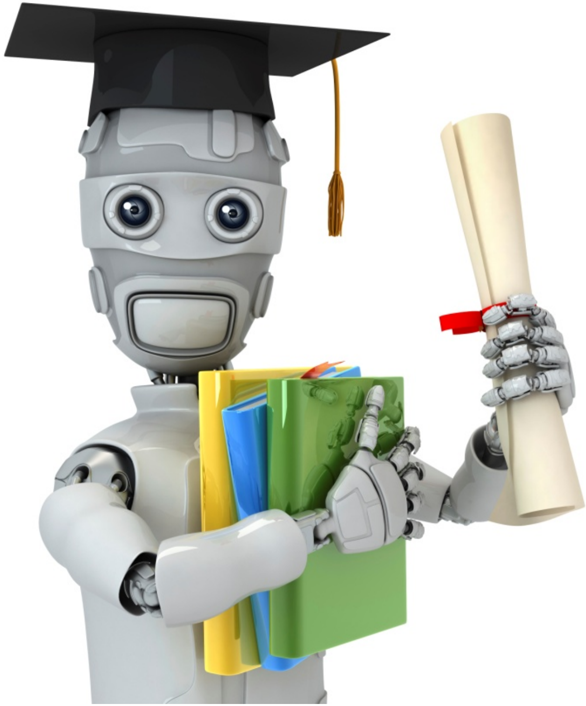


z_1

Country size / GDP

1

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

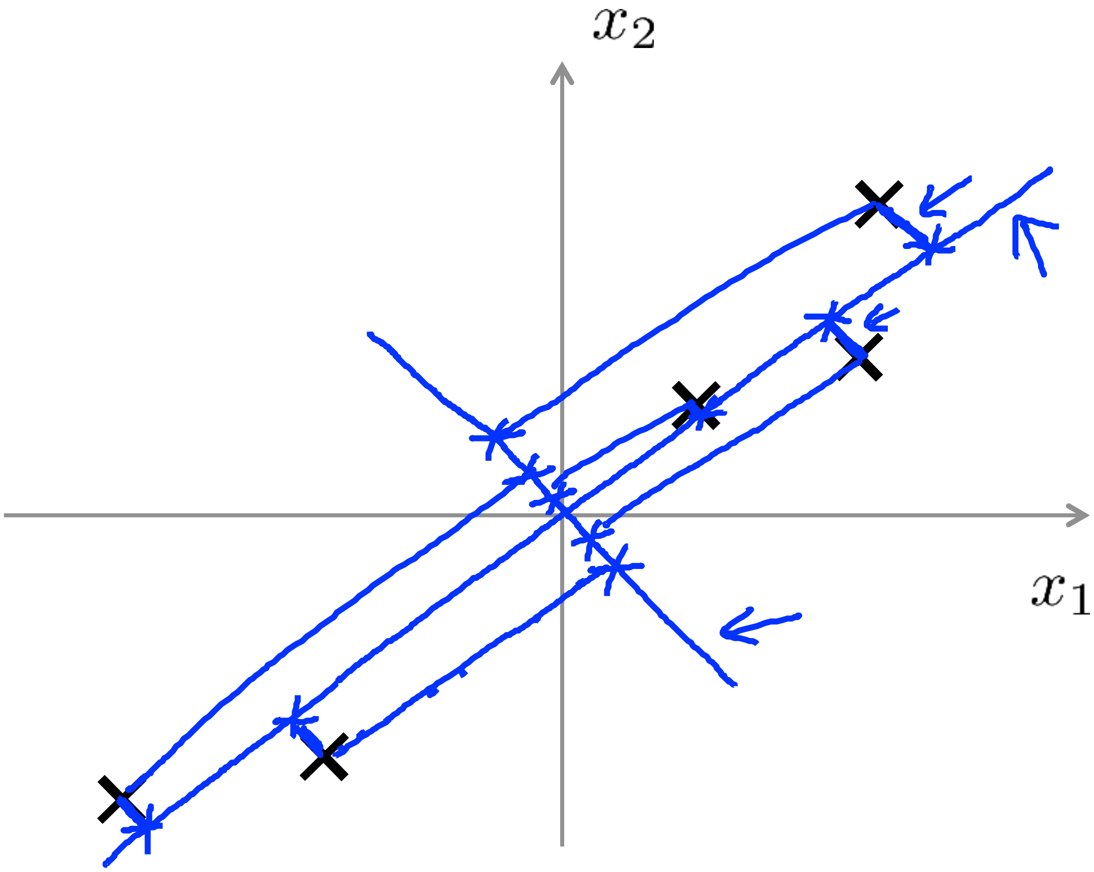


Machine Learning

Dimensionality Reduction

Principal Component Analysis problem formulation

Principal Component Analysis (PCA) problem formulation

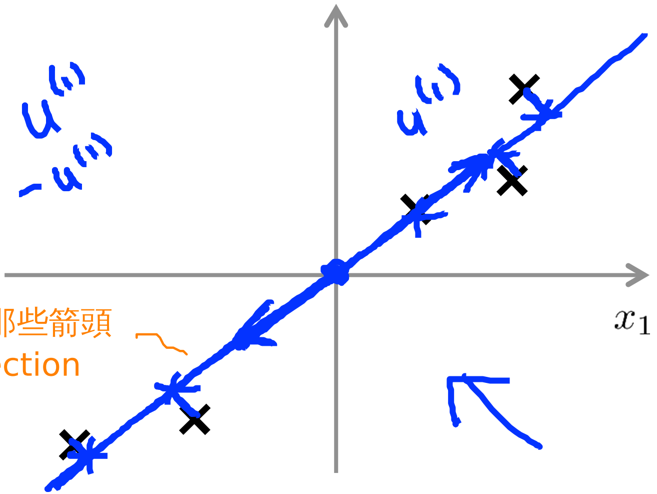


$x \in \mathbb{R}^2$

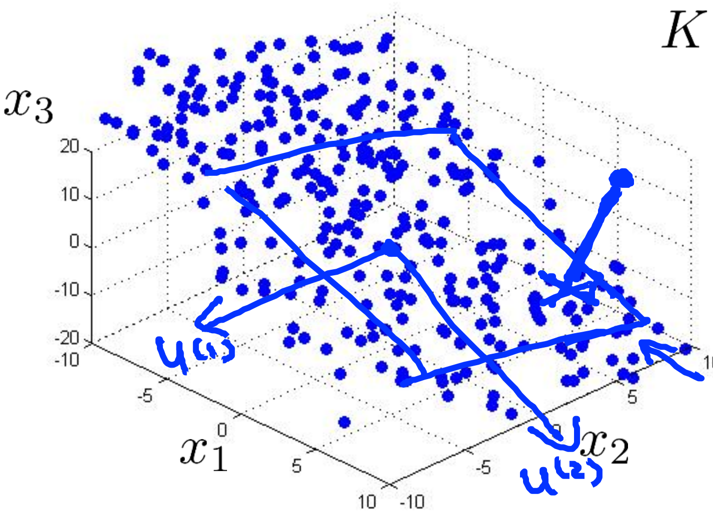
在应用PCA之前 通常的做法是 先进行均值归一化和 特征规范化 使得 特征 x1 和 x2 均值为0 数值在可比较的范围之内(後會詳講)

Principal Component Analysis (PCA) problem formulation

$$3D \rightarrow 2D$$
$$K = 2$$



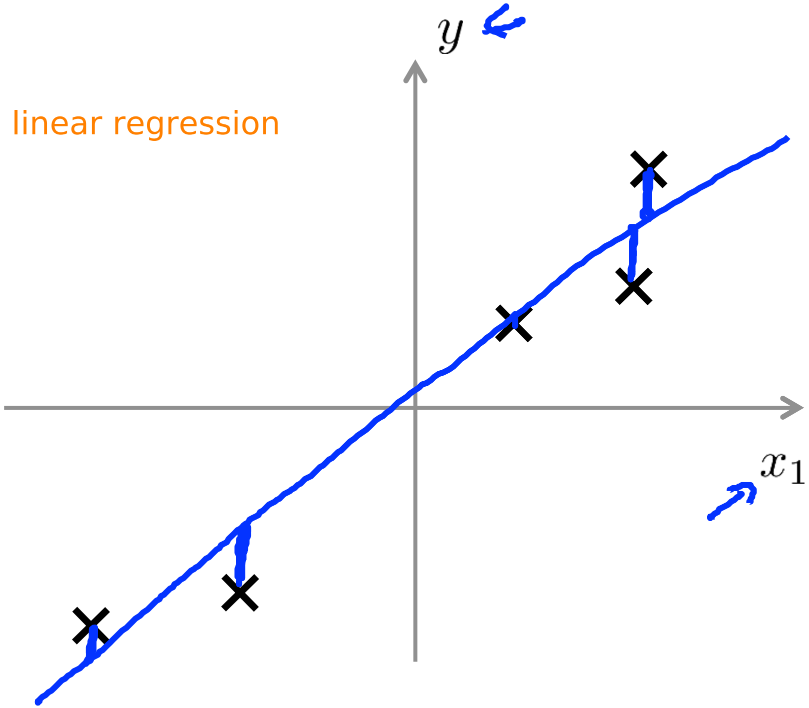
該線上的那些箭頭
就是projection

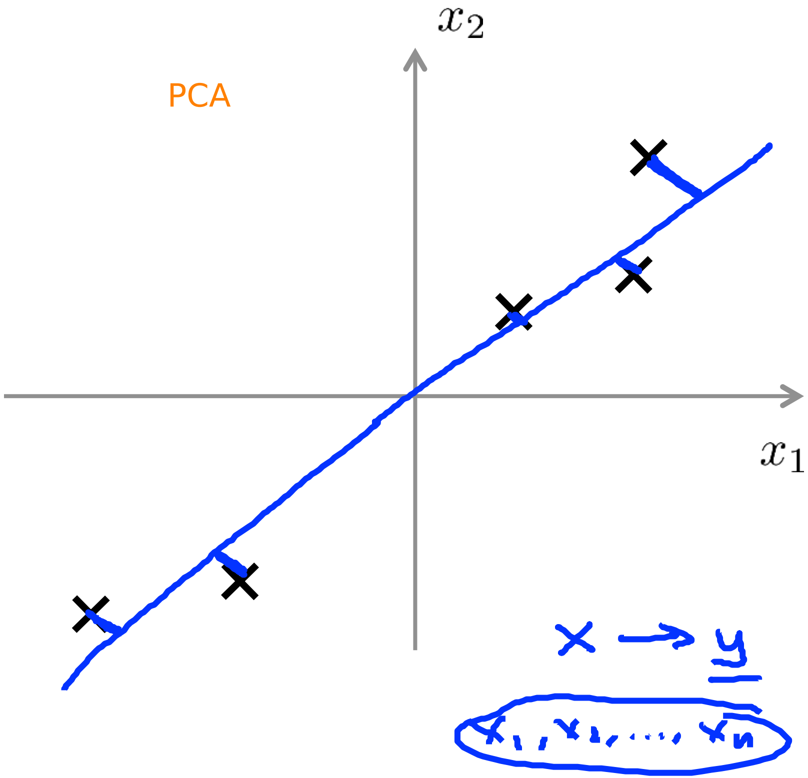


Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

PCA is not linear regression





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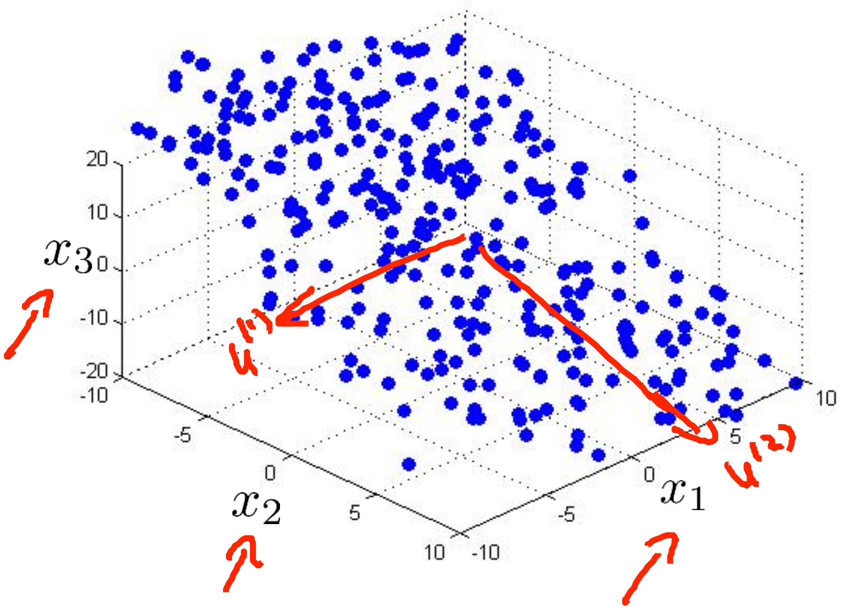
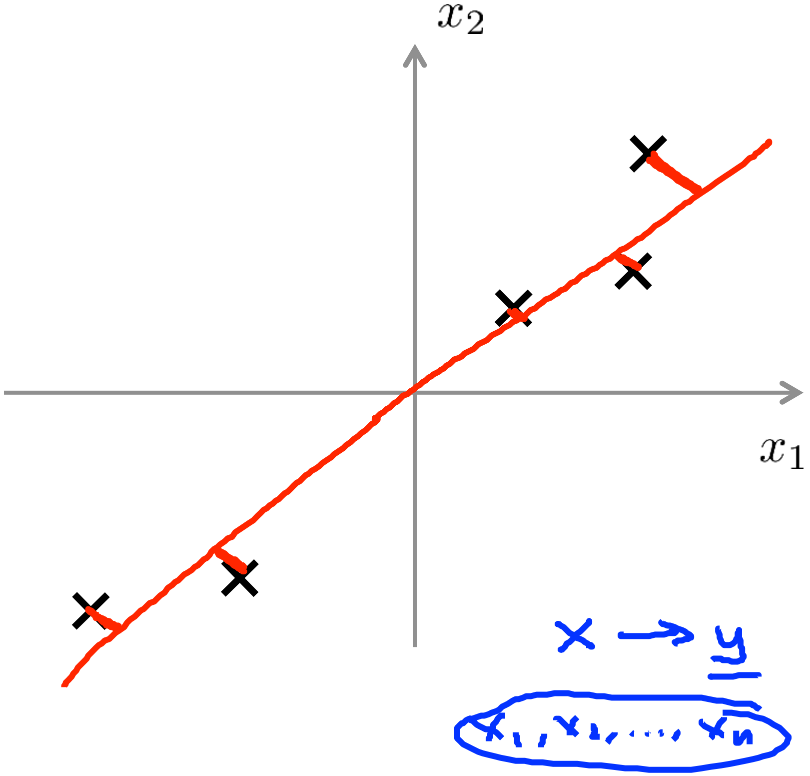
PCA is not linear regression





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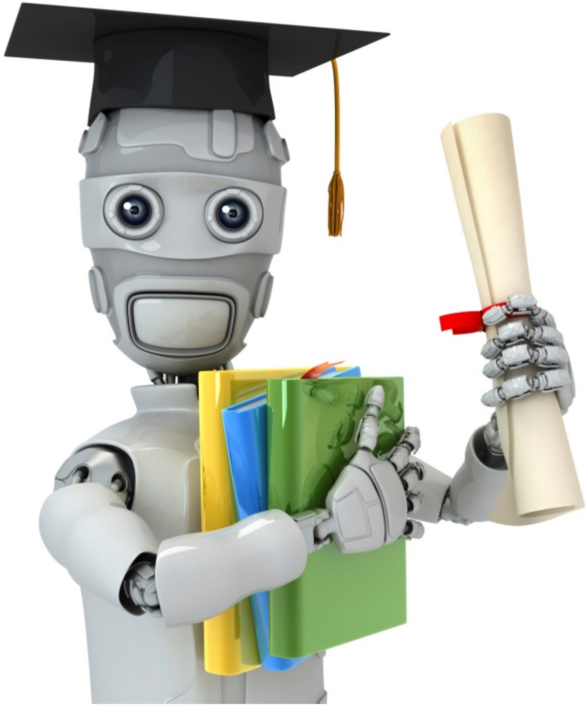


Machine Learning

Dimensionality Reduction

Principal Component Analysis algorithm

Data preprocessing

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

Preprocessing (feature scaling/mean normalization):

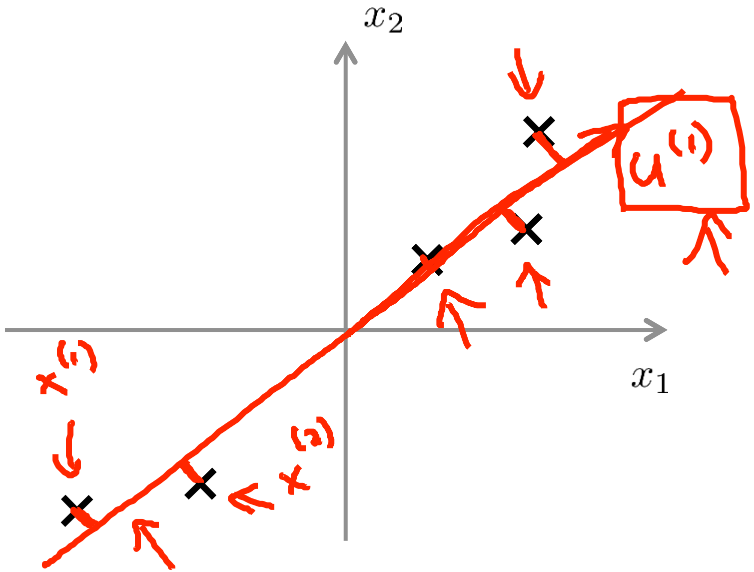
$$\mu_j = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)}$$

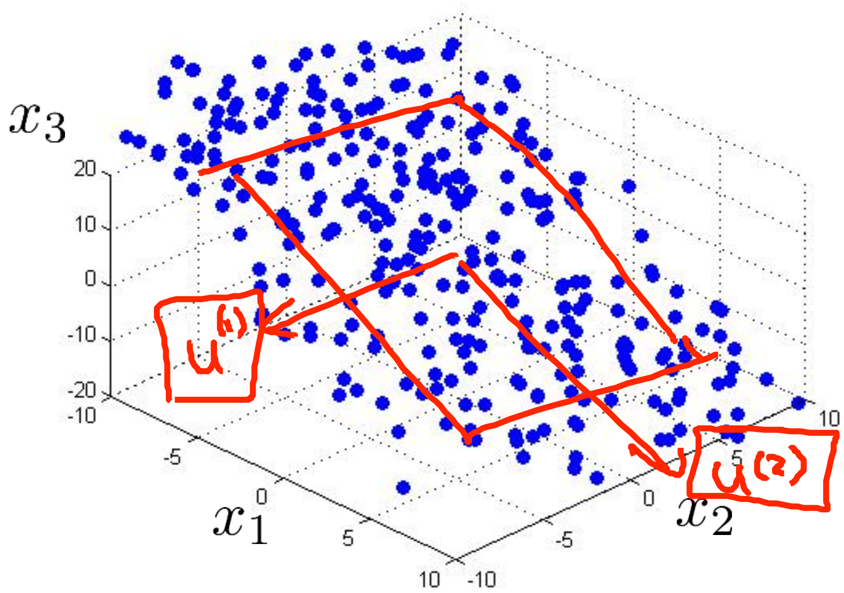
Replace each $x_j^{(i)}$ with $x_j - \mu_j$.

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.

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

Principal Component Analysis (PCA) algorithm



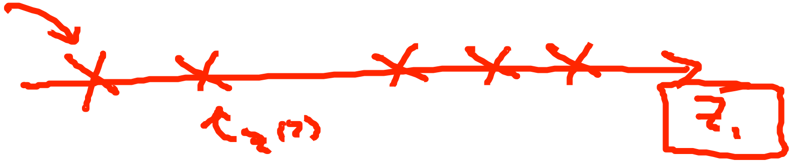


Reduce data from 2D to 1D

Reduce data from 3D to 2D

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

$z^{(i)}$



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

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

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

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

eig(Sigma)

n×n matrix

svd 将输出三个矩阵
分别是 U S V
你真正需要的是 U 矩阵
U 矩阵也是一个
n×n 矩阵
U 矩阵的列就是
我们需要的 u(1) u(2) 等等
如果我们想 将数据的维度从
n 降低到 k 的话
我们只需要提取前 k 列向量

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

k

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

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

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Principal Component Analysis (PCA) algorithm

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

$$\rightarrow U = \left[\begin{array}{cccc} | & | & & | \\ u^{(1)} & u^{(2)} & \ldots & u^{(n)} \\ | & | & & | \end{array}\right] \in \mathbb{R}^{n\times n}$$

$$\underbrace{u^{(1)} \; u^{(2)}}_{k}$$

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

$$z^{(i)} = \underbrace{\underbrace{\left[\begin{array}{cccc} | & | & & | \\ u^{(1)} & u^{(2)} & \ldots & u^{(k)} \\ | & | & & | \end{array}\right]^T}_{n\times k}}_{U_{reduce}} x^{(i)} = \underbrace{\underbrace{\left[\begin{array}{c} —(u^{(1)})^T— \\ \vdots \\ —(u^{(k)})^T— \end{array}\right]}_{k\times n} \underbrace{x^{(i)}}_{n\times 1}}_{k\times 1}$$

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

Principal Component Analysis (PCA) algorithm summary

- After mean normalization (ensure every feature has zero mean) and optionally feature scaling:

$$\texttt{Sigma} = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)})(x^{(i)})^T$$

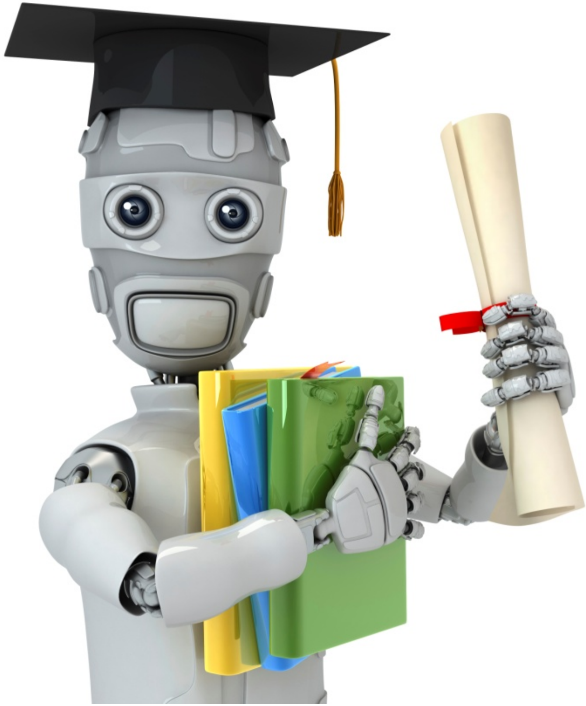
$$X = \begin{bmatrix} — & x^{(1)T} & — \\ & \vdots & \\ — & x^{(m)T} & — \end{bmatrix}$$

$$\boxed{\texttt{Sigma = (1/m) * X' * X;}}$$

```
[U,S,V] = svd(Sigma);
Ureduce = U(:,1:k);
z = Ureduce'*x;
```

$x \in \mathbb{R}^n$ $\cancel{x_0 = 1}$

我没有证明确实能够使得 平方投影误差最小化
证明已经超出了这门课的范围



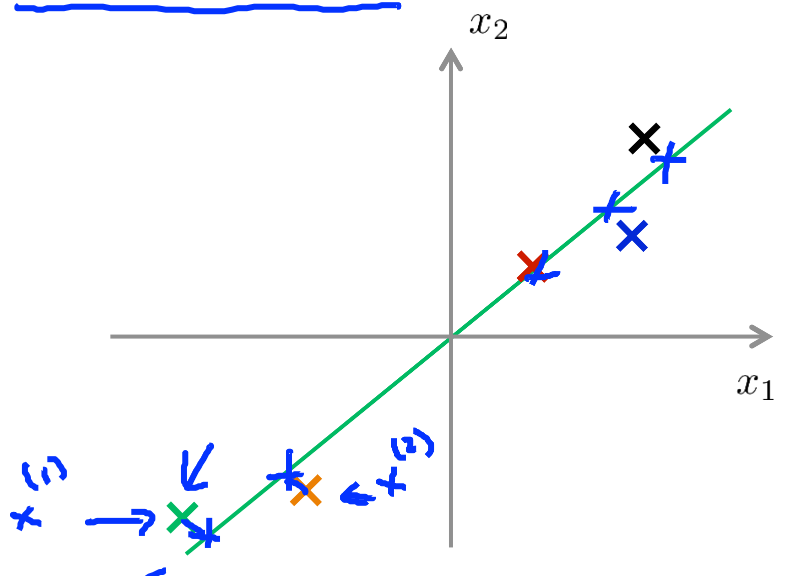
Machine Learning

Dimensionality Reduction

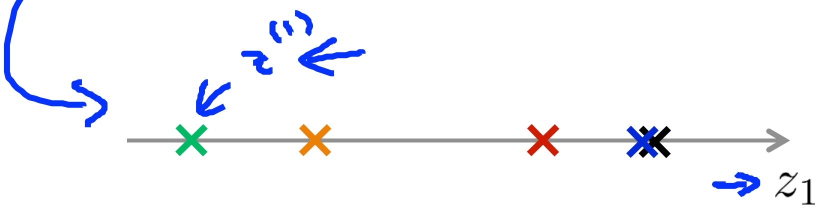
Reconstruction from compressed representation

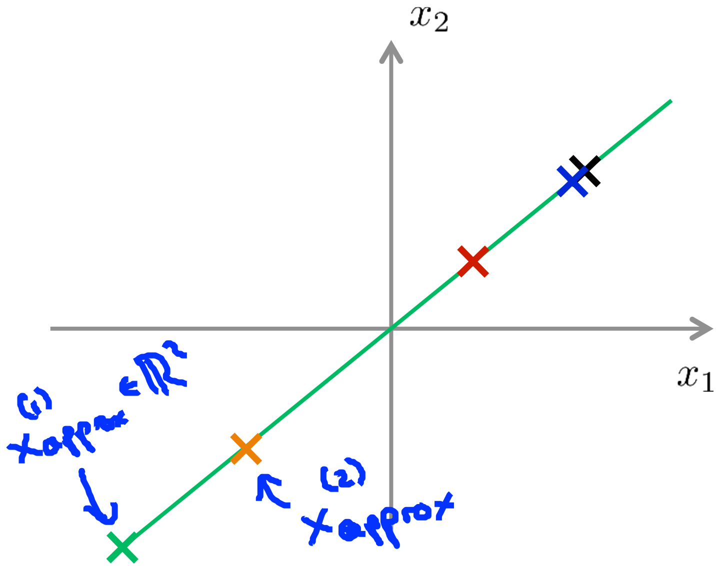
可以从压缩过的数据 近似地回到原始高维度的数据

Reconstruction from compressed representation



$$z = U_{reduce}^T x$$





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

$\tilde{x}$

$$\underbrace{X_{approx}^{(1)}}_{\mathbb{R}^n} = \underbrace{\underbrace{U_{reduce}}_{n \times k} \cdot \underbrace{z^{(1)}}_{k \times 1}}_{n \times 1}$$

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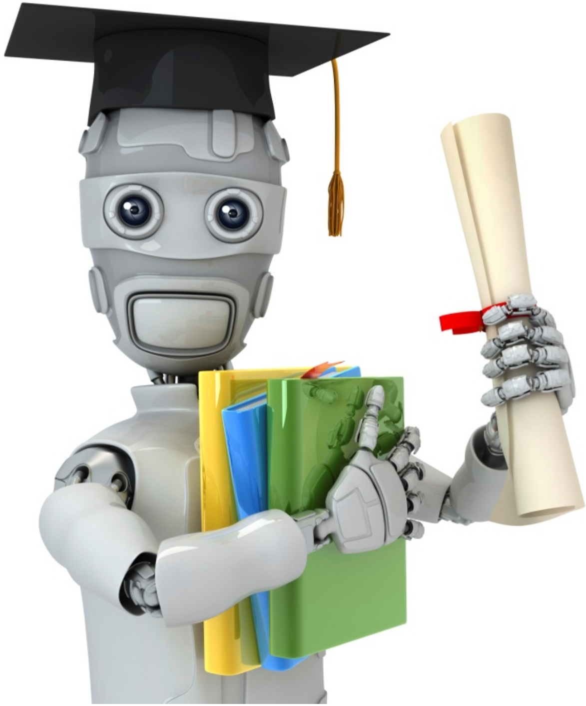


Machine Learning

Dimensionality Reduction

Choosing the number of principal components

Choosing k (number of principal components)

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

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

Typically, choose k to be smallest value so that

$$\rightarrow \frac{\frac{1}{m}\sum_{i=1}^{m} \|x^{(i)} - x_{approx}^{(i)}\|^2}{\frac{1}{m}\sum_{i=1}^{m} \|x^{(i)}\|^2} \leq \cancel{0.01} \quad \cancel{(1\%)}$$

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

0.10 (10%)

→ "~~99%~~ of variance is retained"

~~95%~~ 90%

一个常见的 选择K值的经验法则是 选择能够使得它们之间的比例 小于等于0.01

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

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

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

Choosing k (number of principal components)

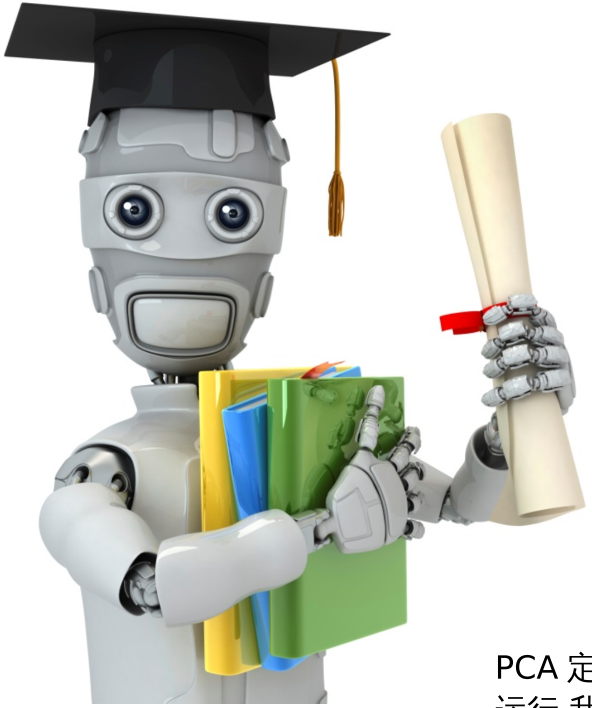
```
[U,S,V] = svd(Sigma)
```

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)



Machine Learning

Dimensionality Reduction

Advice for applying PCA

PCA 定义了从 x到z的对应关系 这种从 x 到 z的对应关系只可以通过 在训练集上
运行 我们需要 使我们的参数唯一地适应 这些训练集 而不是 适应我们的交叉验证
或者测试集 因此Ureduce矩阵中的数据 就应该 只通过对训练集运行PCA来获得
在训练集中找到了 所有这些参数后 就可以 将同样的对应关系应用到其他样本中了
可能 是交叉验证数集样本 或者 用在你的测试数据集中

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

100

100

Supervised learning speedup

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

Extract inputs:

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

$$\downarrow PCA$$

U_{reduce}

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

$x \downarrow z$

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 $x_{test}^{(i)}$ in the cross validation and test sets.

$x \to z$

Application of PCA

(Avado)就分类的精确度而言 数据降维后对学习算法 几乎没有什么影响
如果我们将降维 用在低维数据上 我们的学习算法会运行得更快

- Compression
  - Reduce memory/disk needed to store data
  - Speed up learning algorithm

Choose k by % of variance retain

- Visualization

k=2 or k=3

Bad use of PCA: To prevent overfitting

→ Use $z^{(i)}$ instead of $x^{(i)}$ to reduce the number of features to $k < n$. — 10000

1000

Thus, fewer features, less likely to overfit.

如果你仔细想想PCA是如何工作的 它并不需要使用数据的标签
PCA做了什么呢 它把某些信息舍弃掉了

Bad!

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

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

同时正则化 效果也会比PCA更好
总之 使用PCA的目的是 加速 学习算法的时候是好的
但是用它来避免过拟合 却并不是一个好的PCA应用

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 $\{(\cancel{z^{(1)}}\, x^{(i)}, y^{(1)}), \ldots, (\cancel{z^{(m)}}\, x^{(m)}, y^{(m)})\}$
- 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 $\underline{z^{(i)}}$.