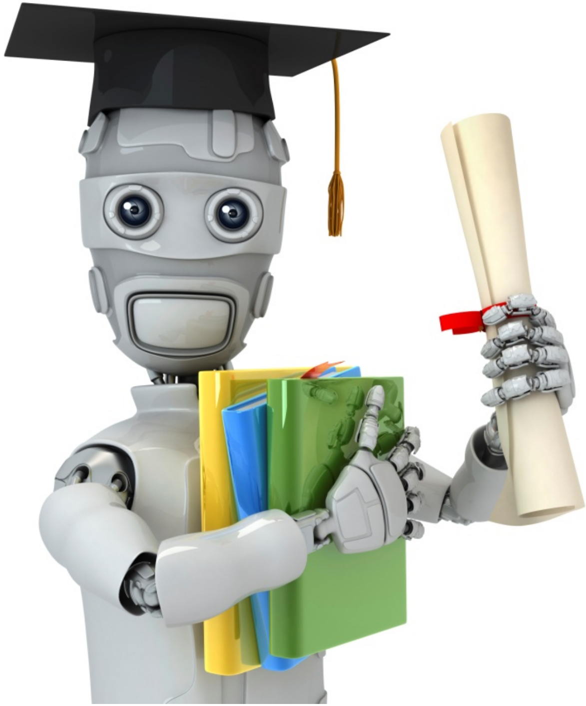
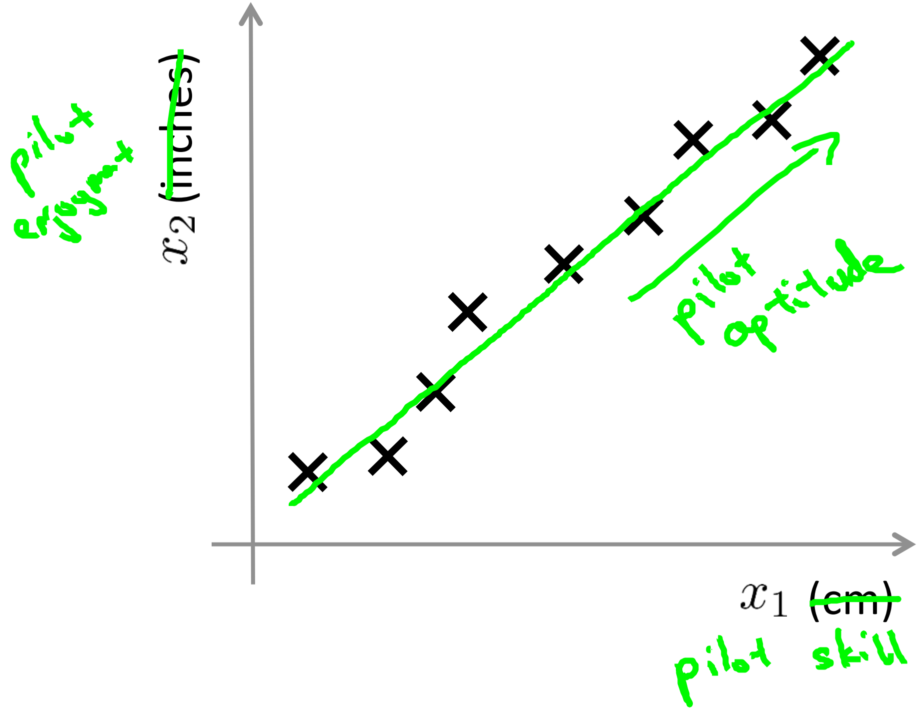


Machine Learning

Dimensionality Reduction

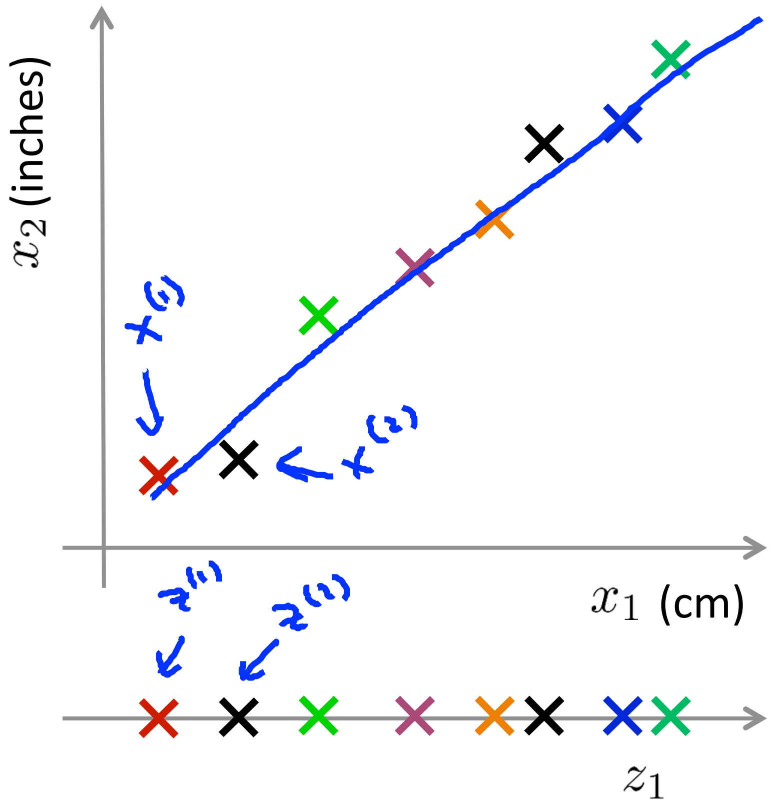
Motivation I: Data Compression

Data Compression



Reduce data from 2D to 1D

Data Compression



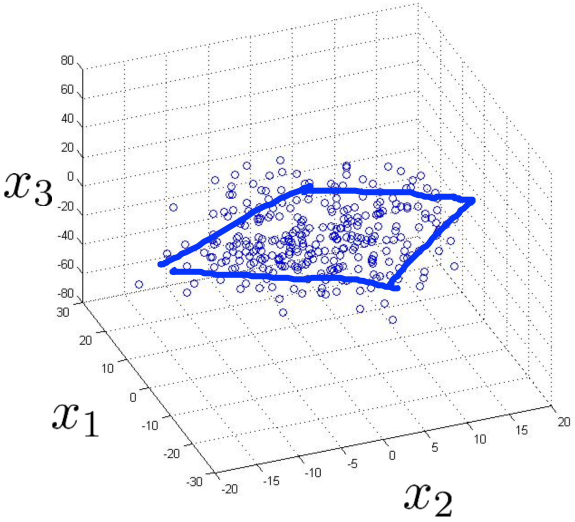
Reduce data from 2D to 1D

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

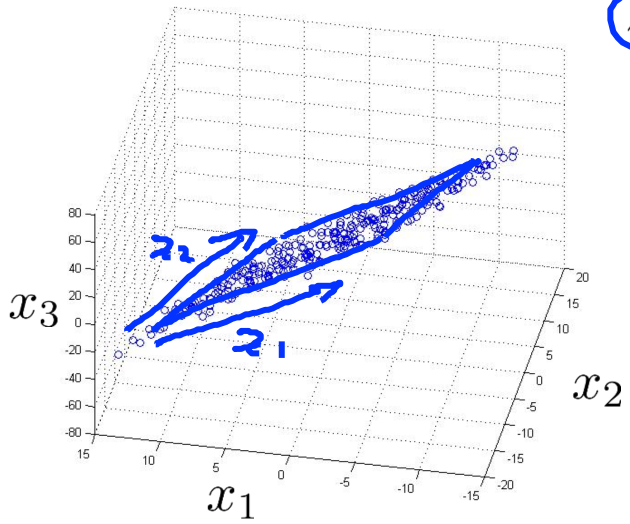
Data Compression

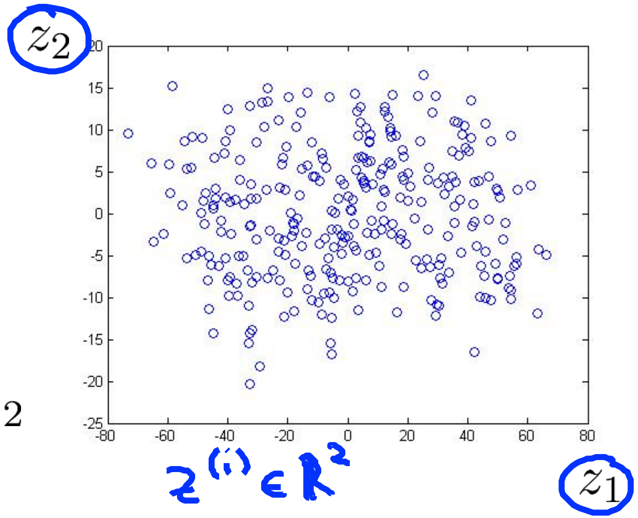
$1000D \rightarrow 100D$

Reduce data from 3D to 2D



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

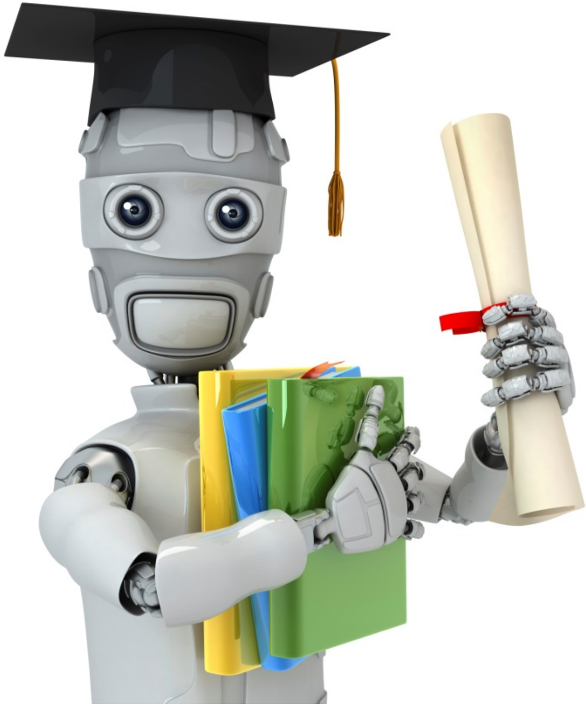




$z^{(i)} \in \mathbb{R}^2$

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

Andrew Ng



Machine Learning

Dimensionality Reduction

Motivation II: Data Visualization

Data Visualization

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

	x_1	x_2	x_3	x_4	x_5	x_6	
Country	GDP (trillions of US$)	Per capita GDP (thousands of intl. $)	Human Development Index	Life expectancy	Poverty Index (Gini as percentage)	Mean household income (thousands of US$)	…
→ 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]

Data Visualization

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

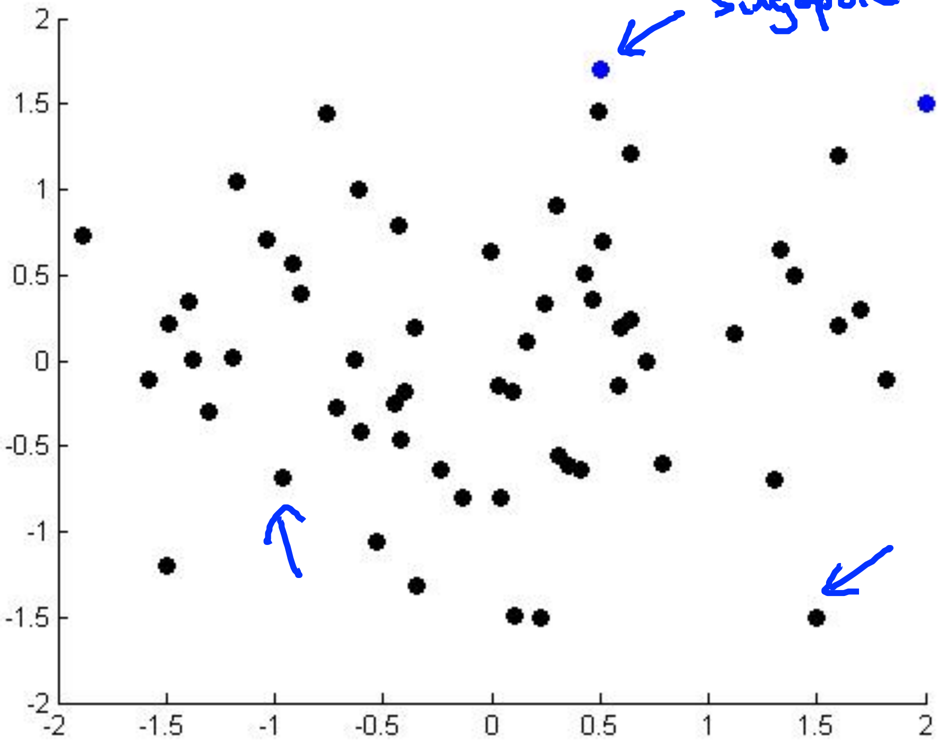
Country	z_1	z_2
Canada	1.6	1.2
China	1.7	0.3
India	1.6	0.2
Russia	1.4	0.5
Singapore	0.5	1.7
USA	2	1.5
…	…	…

Reduce data from 50D to 2D

Data Visualization

per. person GDP (economic activity)

z_2



Singapore

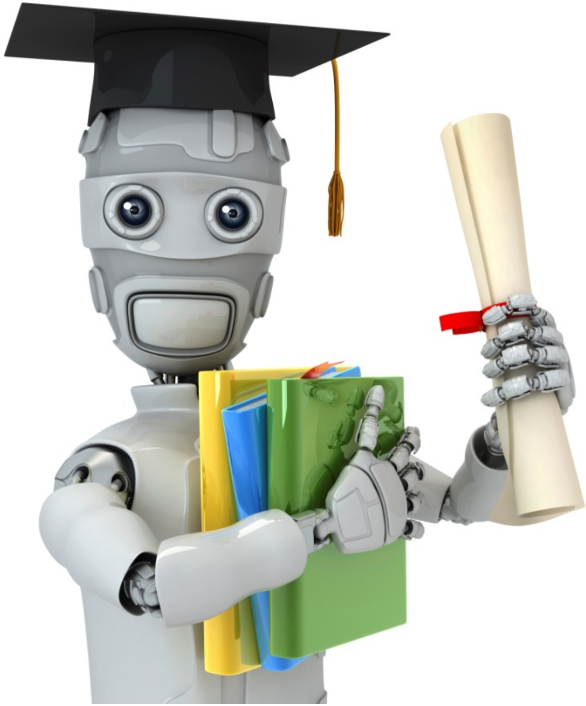
USA

z_1

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

Country size / GDP

1

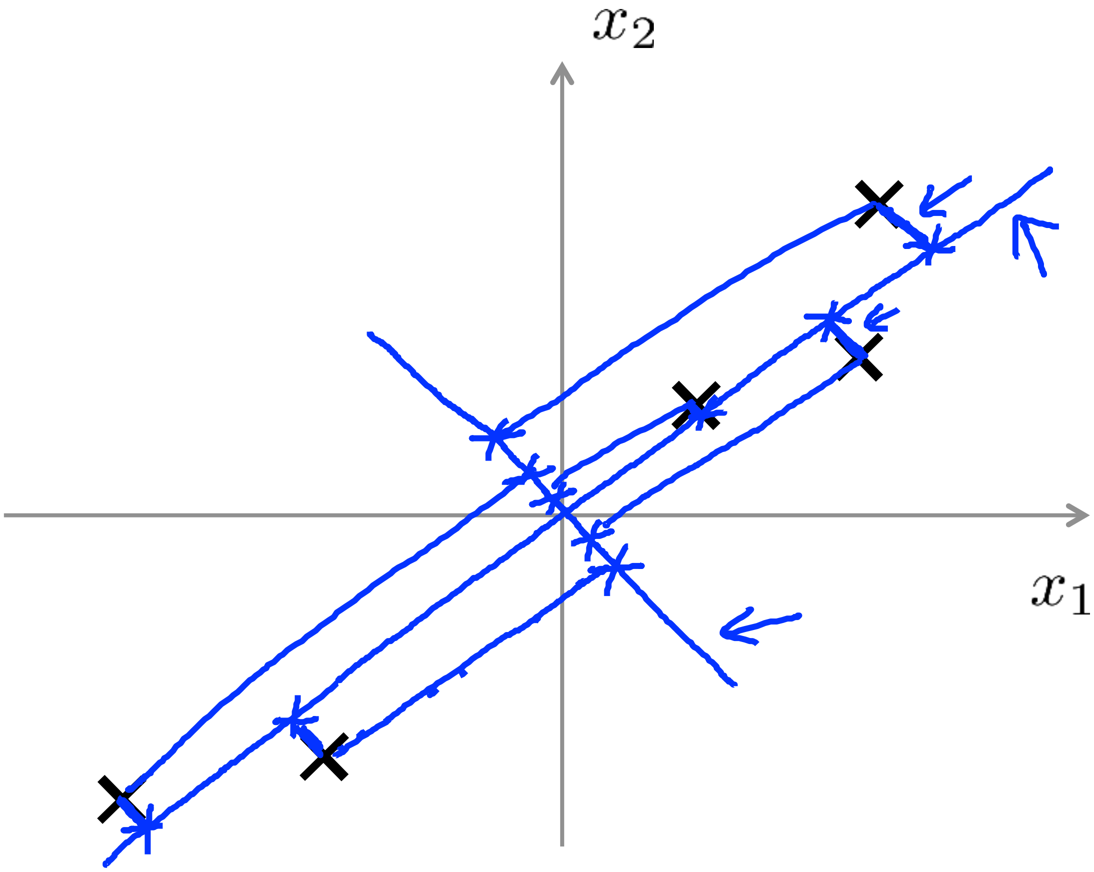


Machine Learning

Dimensionality Reduction

Principal Component Analysis problem formulation

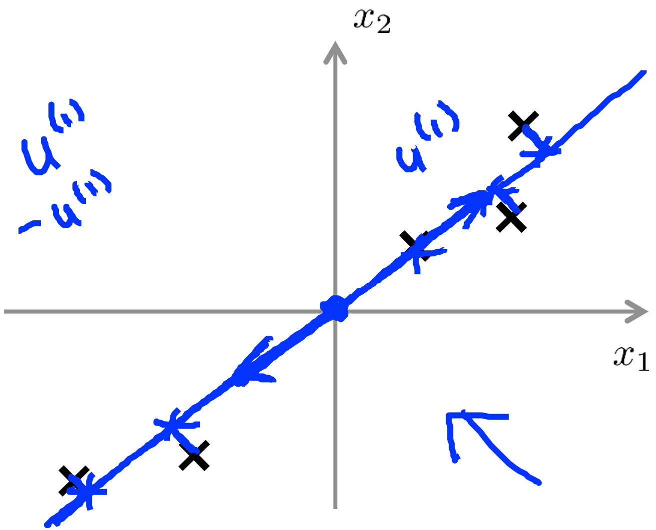
Principal Component Analysis (PCA) problem formulation

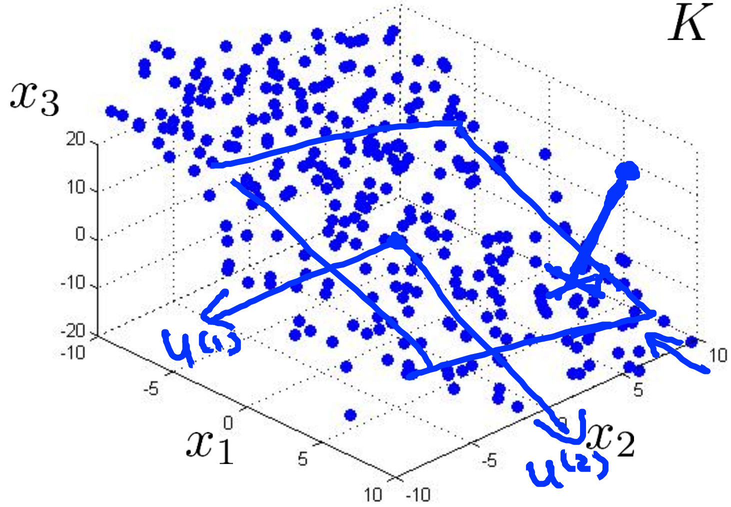


$x \in \mathbb{R}^2$

Principal Component Analysis (PCA) problem formulation

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

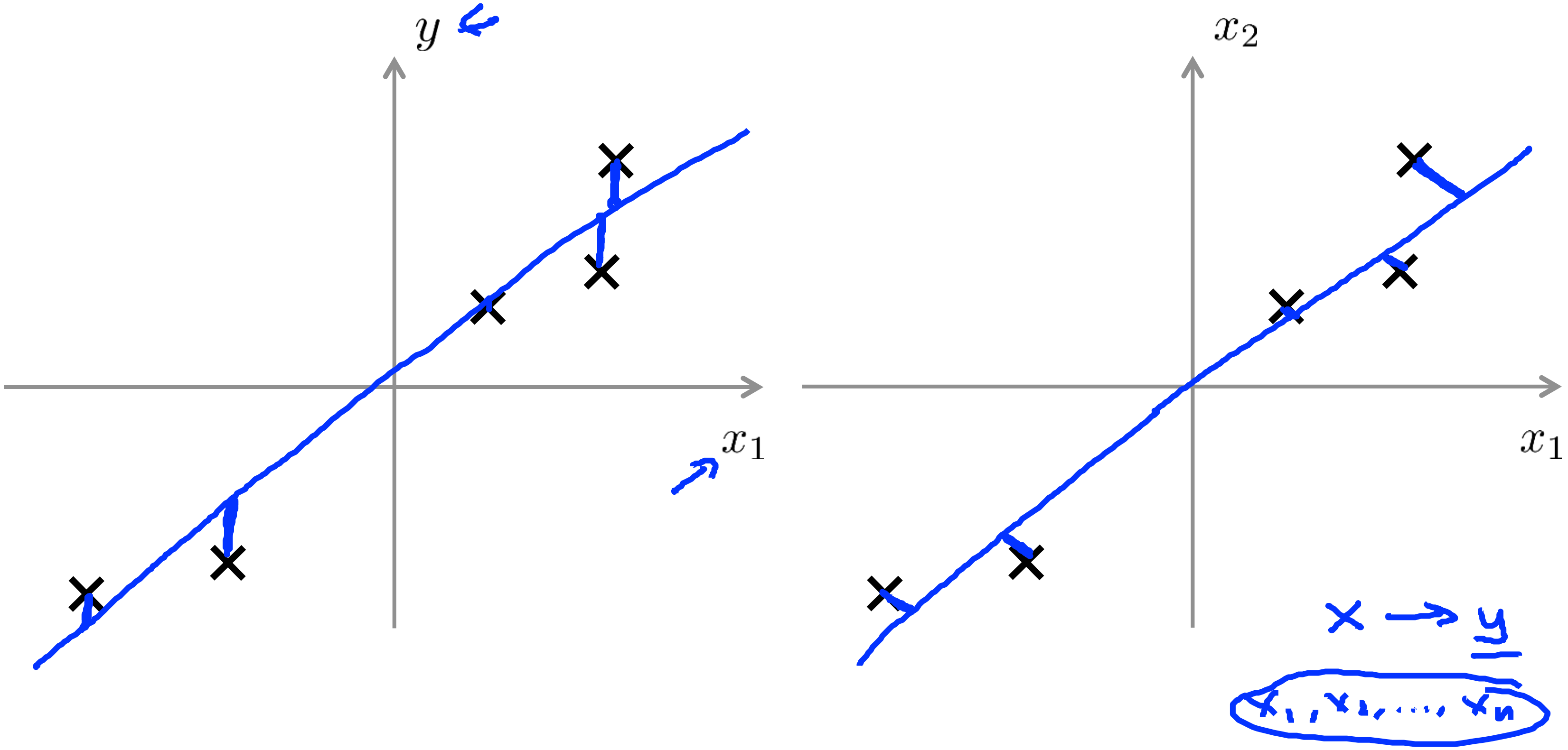




Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

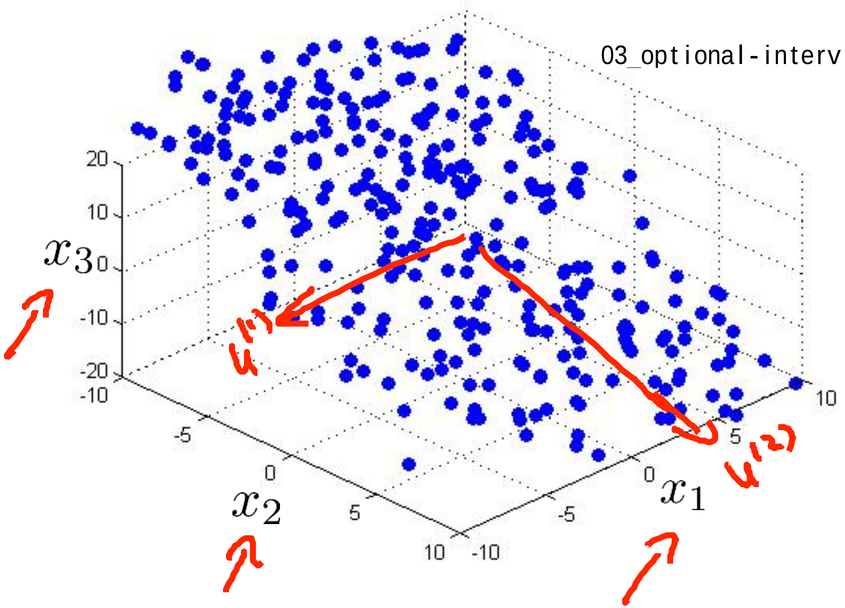
Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

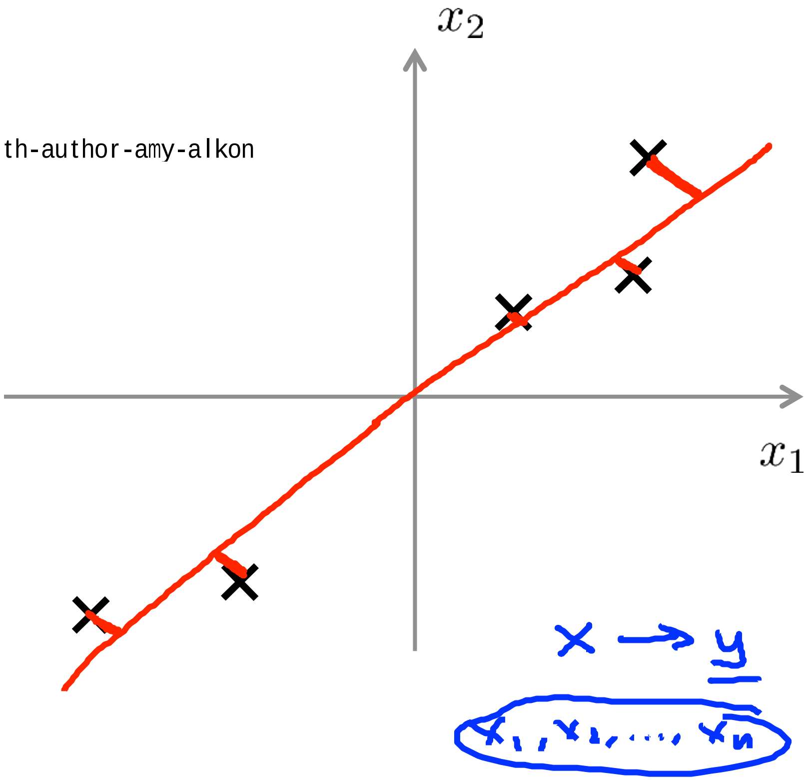
PCA is not linear regression

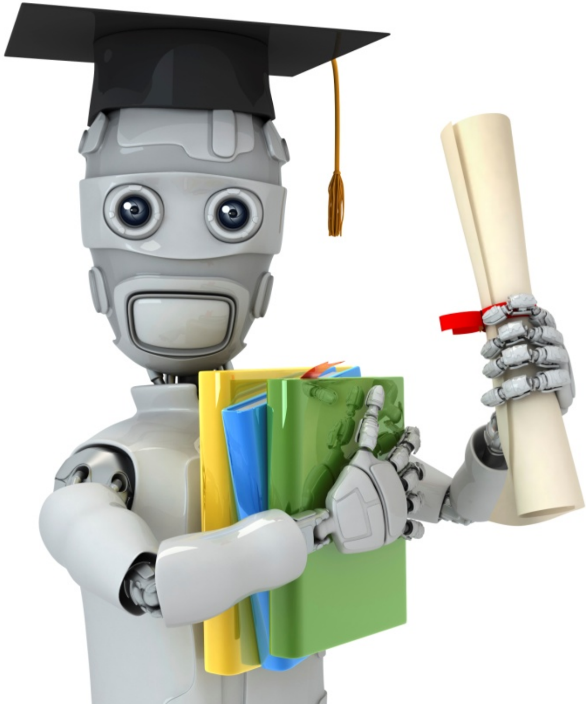


PCA is not linear regression

03_optional-interview-with-author-amy-alkon







Machine Learning

Dimensionality Reduction

Principal Component Analysis algorithm

Data preprocessing

数据预处理

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

Preprocessing (feature scaling/mean normalization):

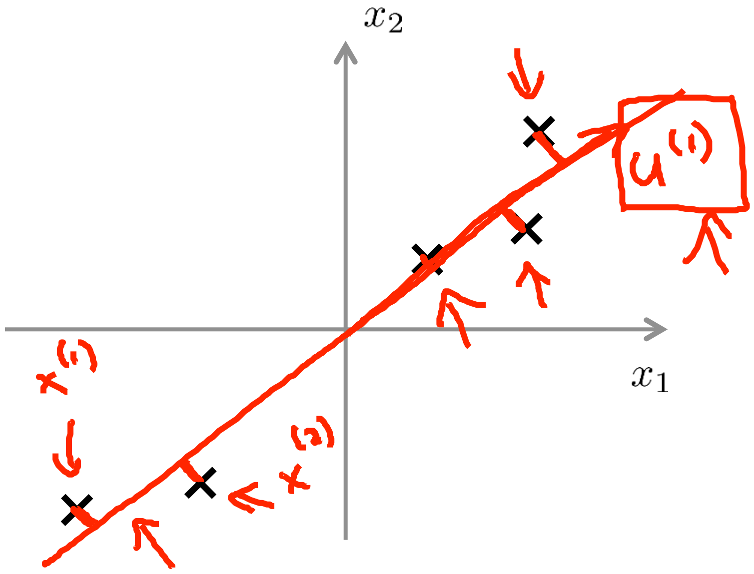
$$\mu_j = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)}$$

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.

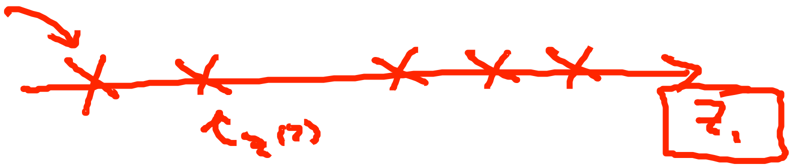
$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j}$$

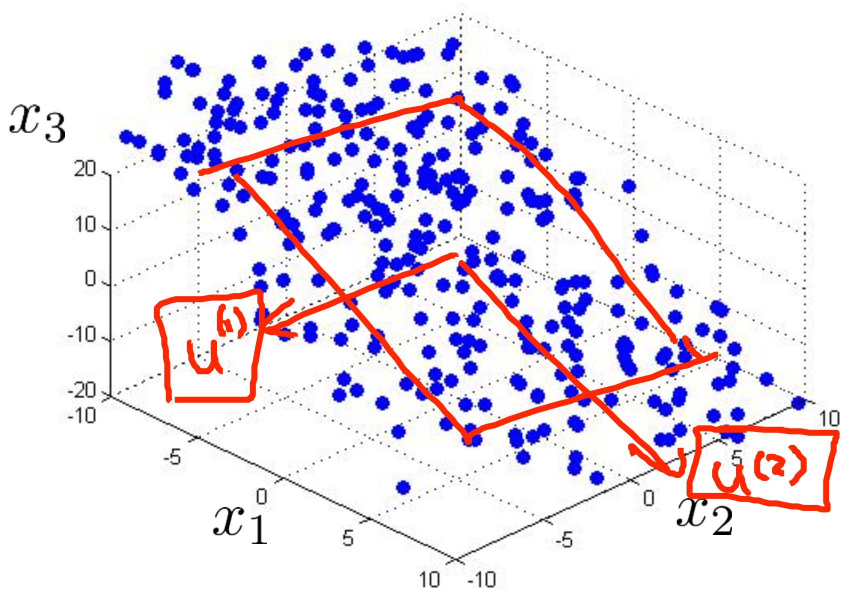
Principal Component Analysis (PCA) algorithm



Reduce data from 2D to 1D

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





Reduce data from 3D to 2D

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

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

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 :

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

n×n matrix

→ Singular value decomposition

eig(Sigma)

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

k

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

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

Principal Component Analysis (PCA) algorithm

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

使用计算出来的前k列去降维

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

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

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

U_{reduce}

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

Principal Component Analysis (PCA) algorithm summary

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

```
Sigma =
```

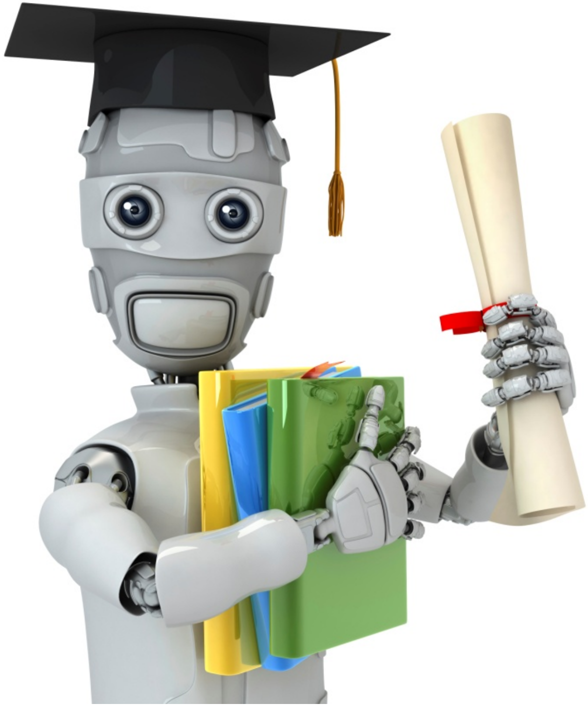
$$\frac{1}{m}\sum_{i=1}^{m}(x^{(i)})(x^{(i)})^T$$

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

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

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

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

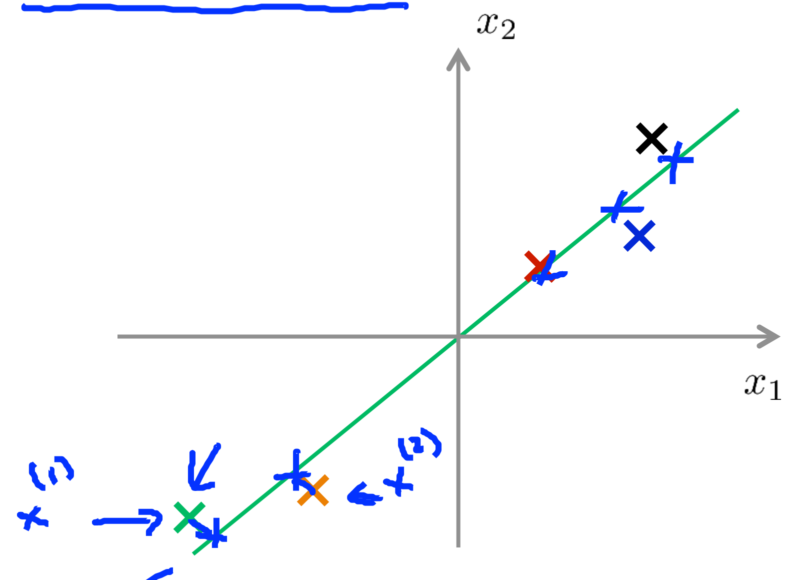


Machine Learning

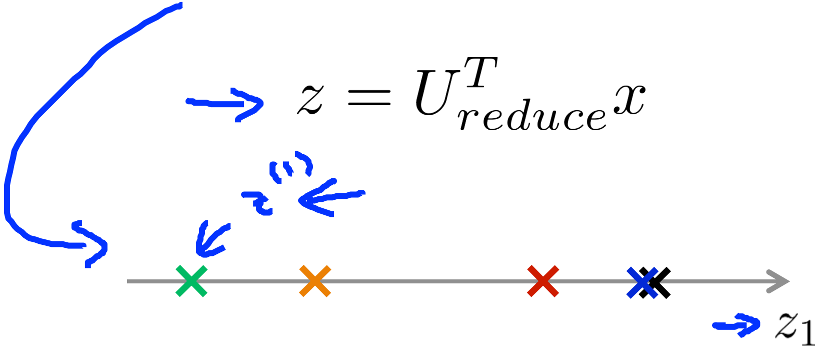
Dimensionality Reduction

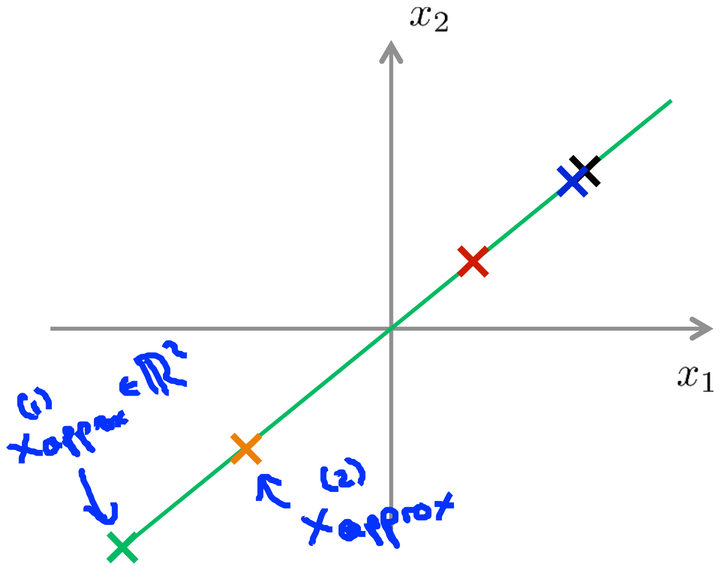
Reconstruction from compressed representation

Reconstruction from compressed representation



$$\rightarrow \quad z = U_{reduce}^T x$$



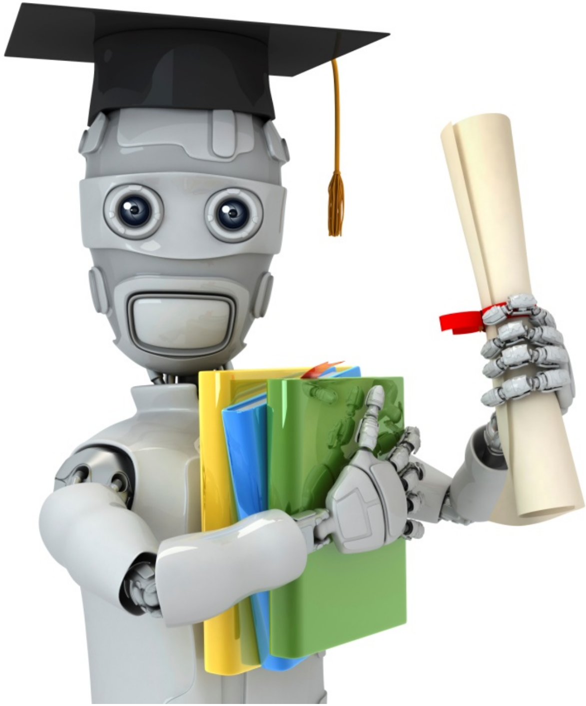


$$z \in \mathbb{R} \rightarrow x \in \mathbb{R}^2$$

$$\tilde{x} \quad x^{(1)}_{approx} = \underbrace{\underbrace{U_{reduce}}_{n \times k} \cdot \underbrace{z^{(1)}}_{k \times 1}}_{n \times 1}$$

$\in \mathbb{R}^n$

Andrew Ng



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

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

~~0.05~~ ~~5%~~

0.10 (10%)

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

~~95%~~ 90%

Andrew Ng

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

$[U, \boxed{S}, V] = \texttt{svd(Sigma)}$

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

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)

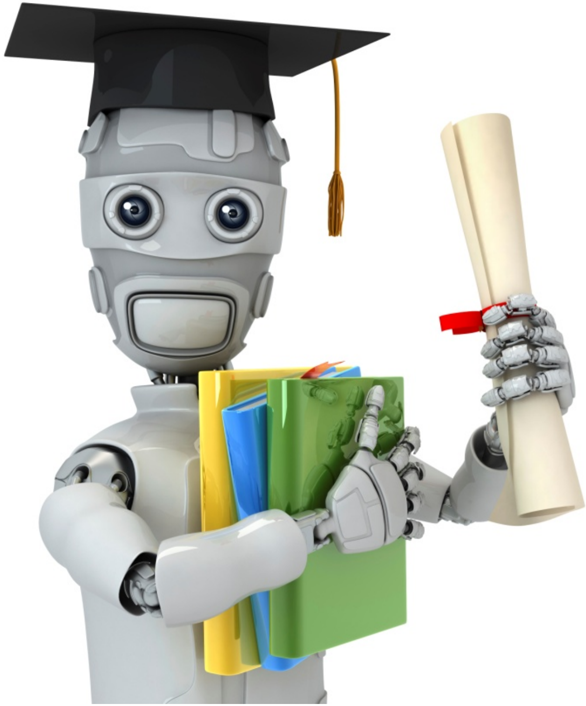
```
[U,S,V] = svd(Sigma)
```

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

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

$$\downarrow PCA$$

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

$x \downarrow z$

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

$x \rightarrow z$

Application of PCA

- 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 $\overset{1000}{k} < n$. — 10000
Thus, fewer features, less likely to overfit.

Bad!

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

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

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 $z^{(i)}$.