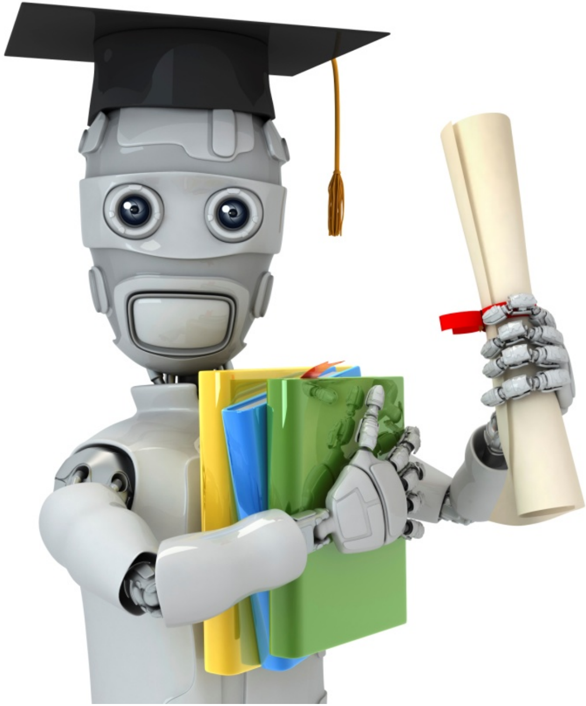
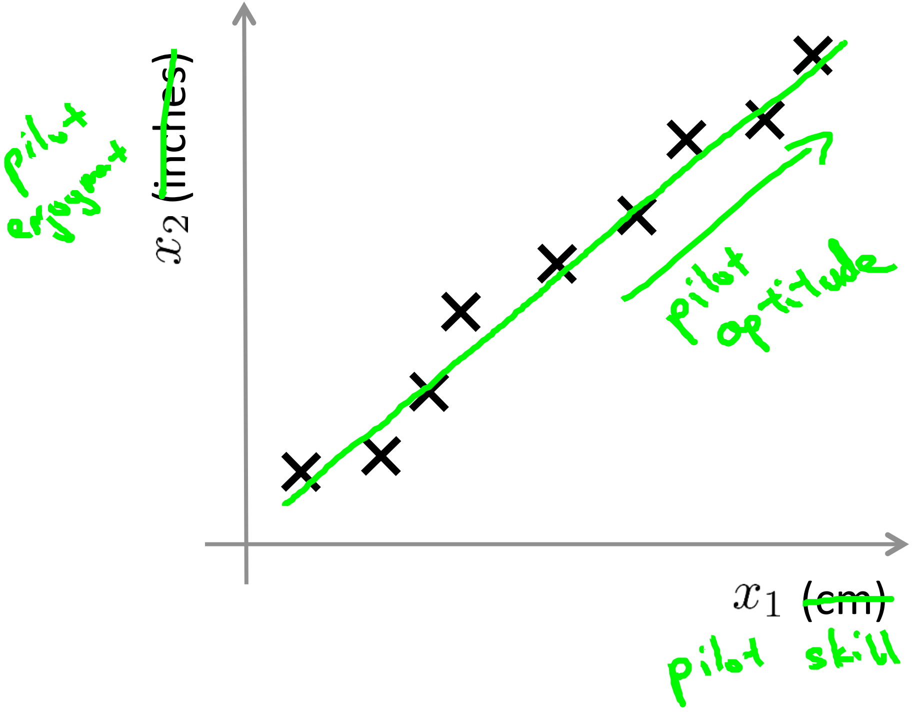


Machine Learning

Dimensionality Reduction

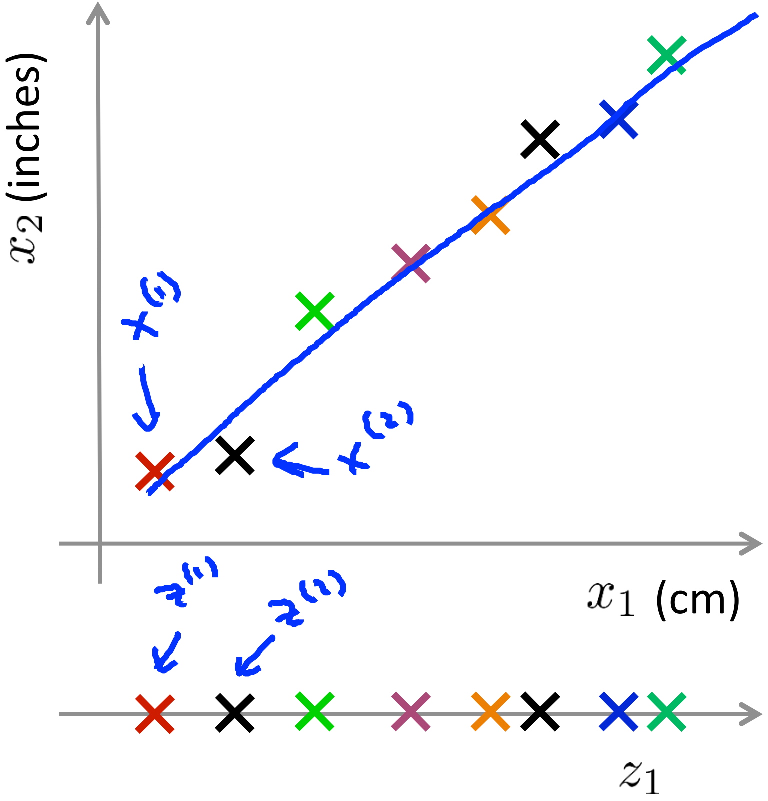
Motivation I: Data Compression

Data Compression



Reduce data from 2D to 1D

Data Compression



Reduce data from 2D to 1D

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

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

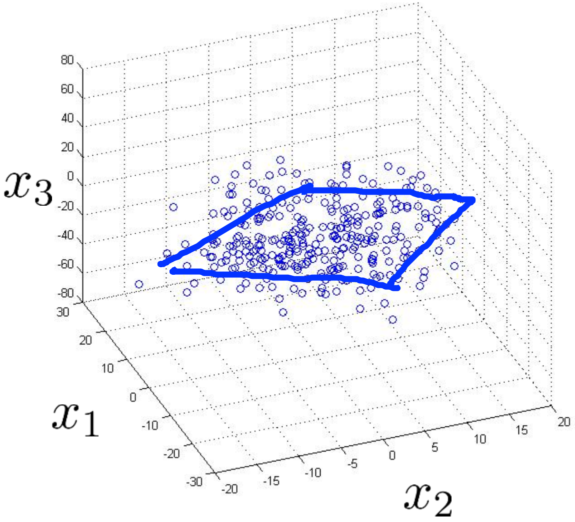
$\vdots$

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

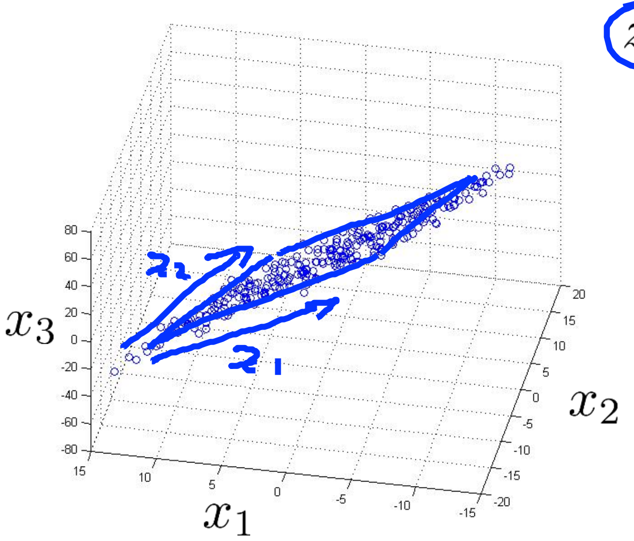
Data Compression

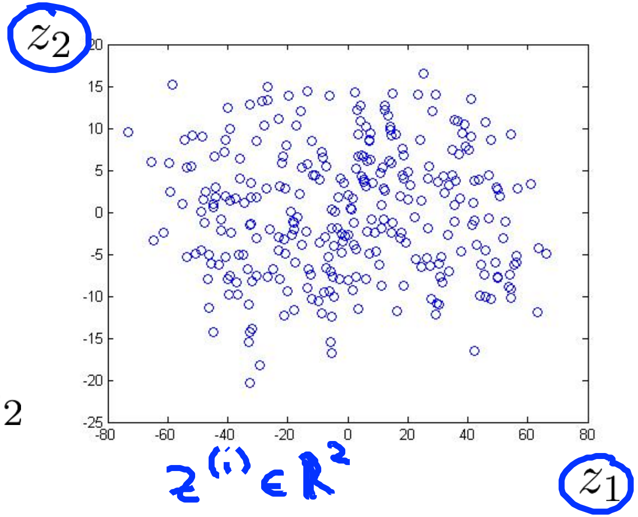
1000D → 100D

Reduce data from 3D to 2D



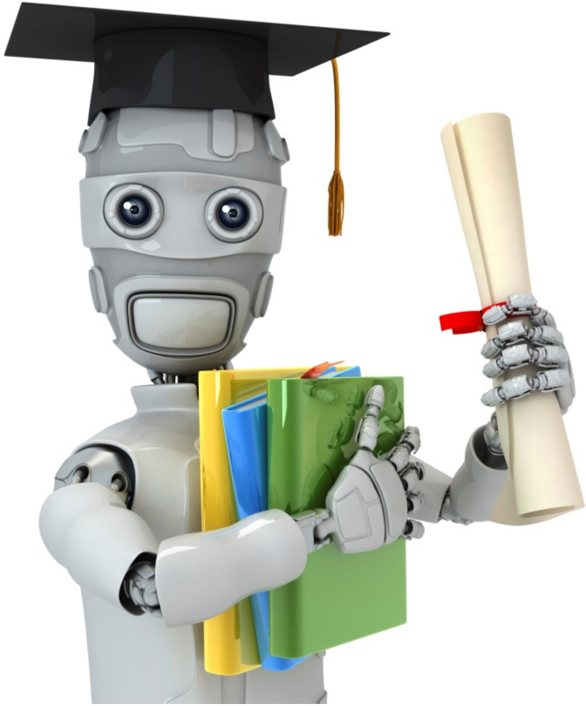
$x^{(i)} \in \mathbb{R}^3$





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

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



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]

Data Visualization

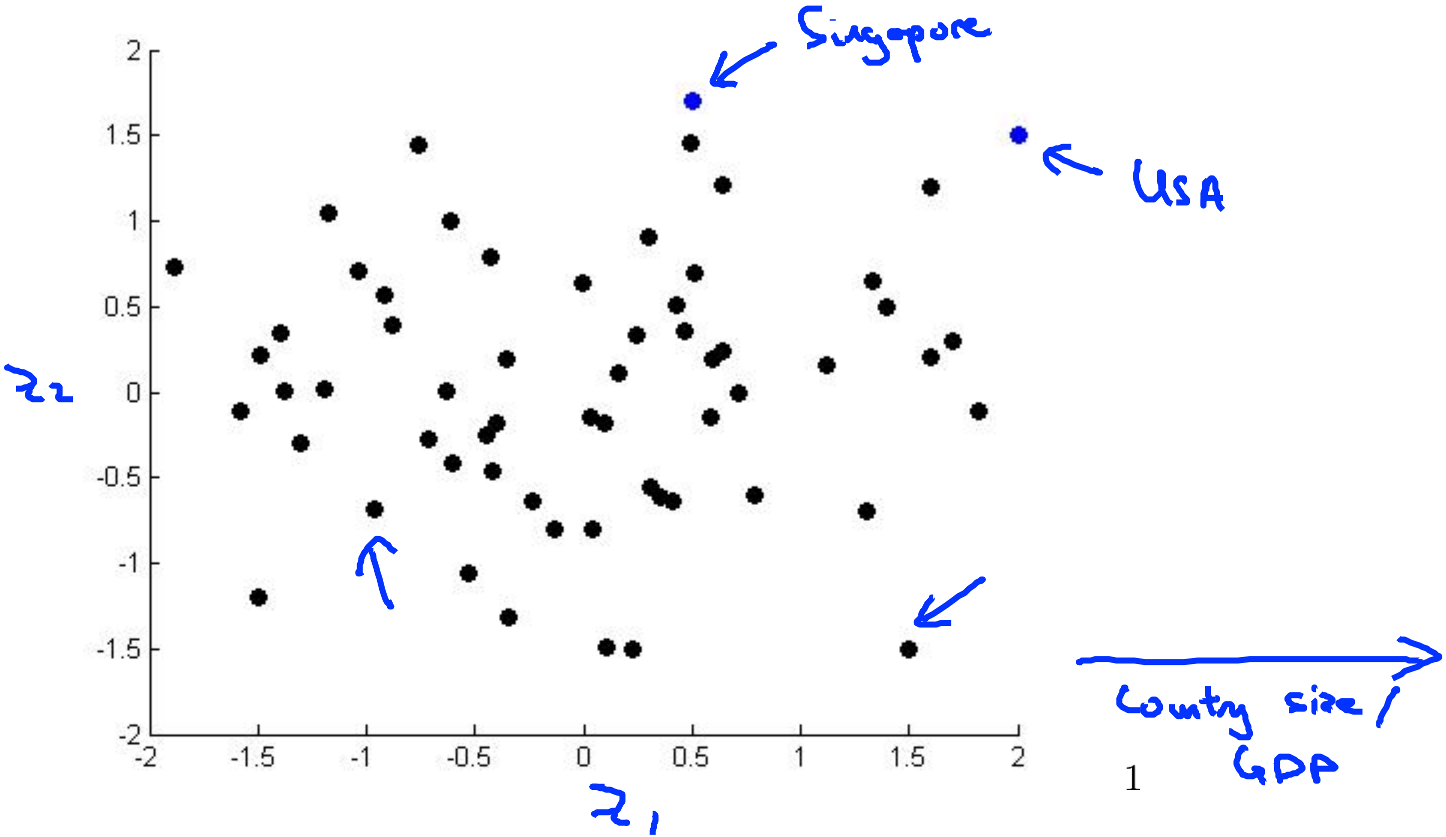
Country	z_1	z_2
Canada	1.6	1.2
China	1.7	0.3
India	1.6	0.2
Russia	1.4	0.5
Singapore	0.5	1.7
USA	2	1.5
…	…	…

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

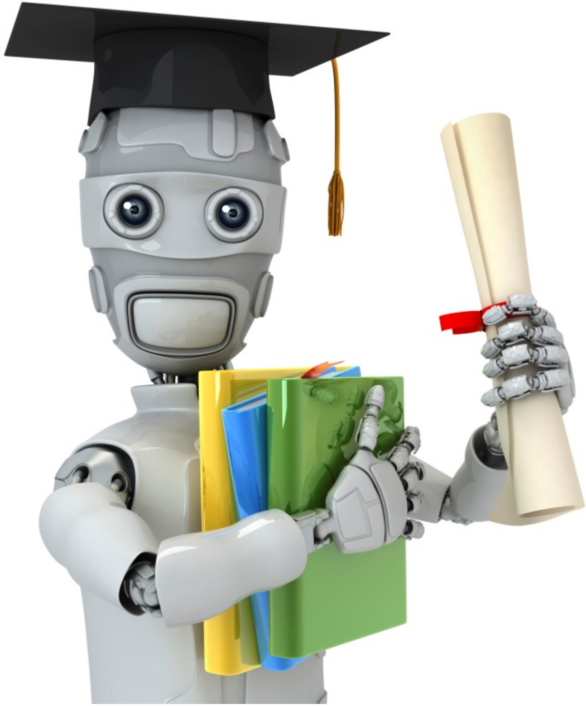
Reduce data from 50D to 2D

Data Visualization

per. person GDP (economic activity)



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

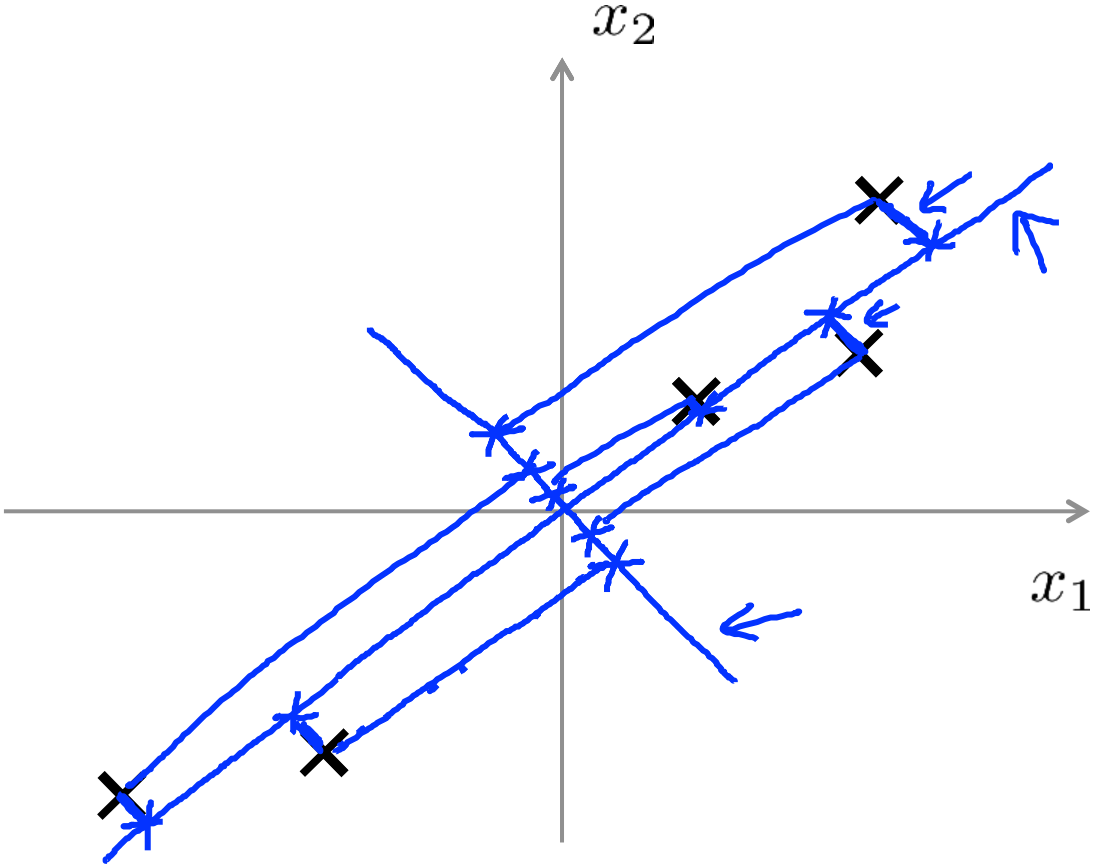


Machine Learning

Dimensionality Reduction

Principal Component Analysis problem formulation

Principal Component Analysis (PCA) problem formulation

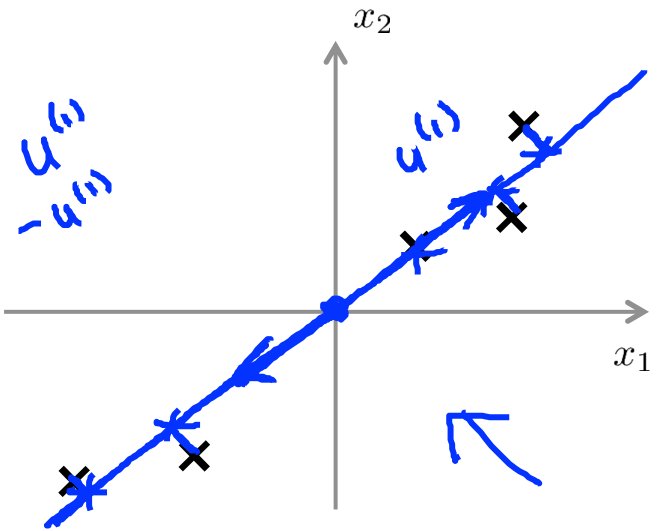


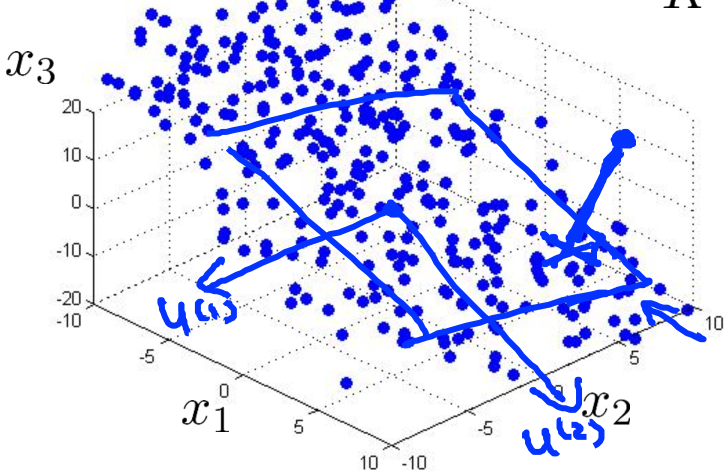
$x \in \mathbb{R}^2$

Andrew Ng

Principal Component Analysis (PCA) problem formulation

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

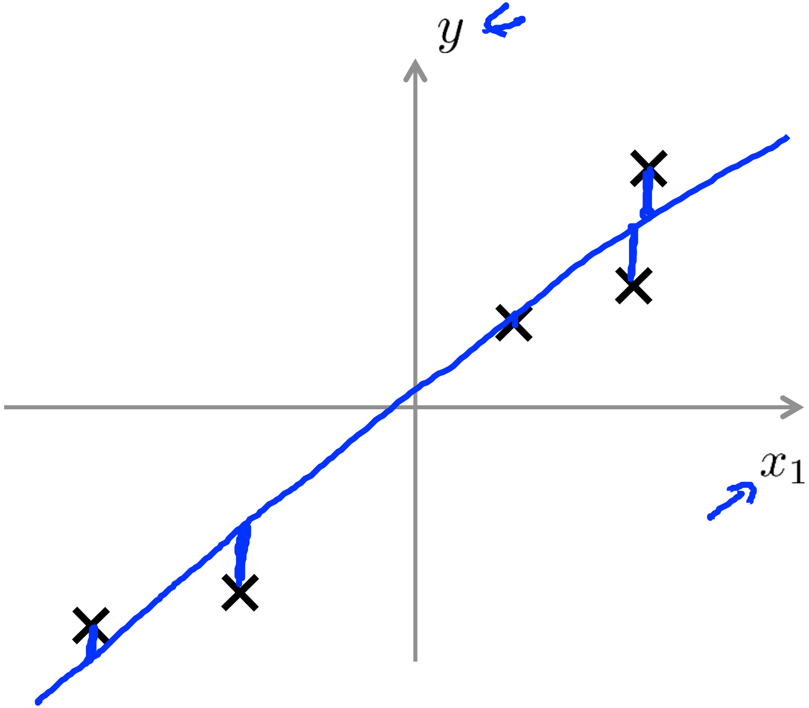


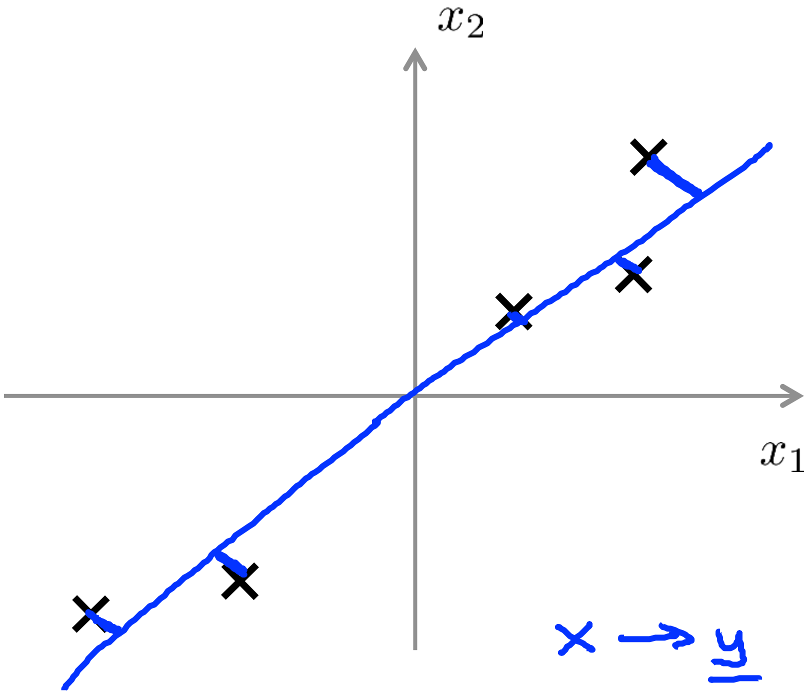


Reduce from 2-dimension to 1-dimension: Find a direction (a vector $\underline{u^{(1)} \in \mathbb{R}^n}$) onto which to project the data so as to minimize the projection error.

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

PCA is not linear regression

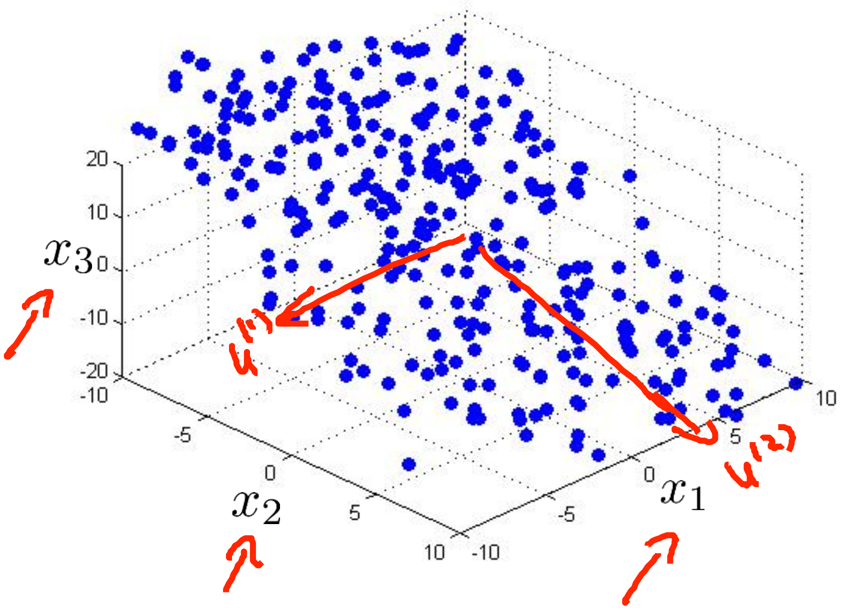


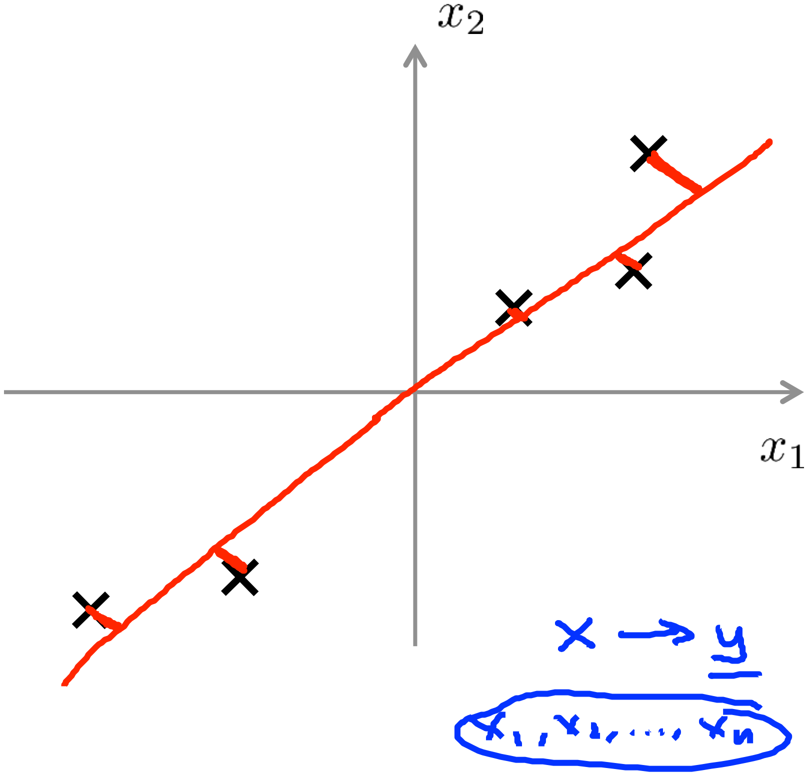


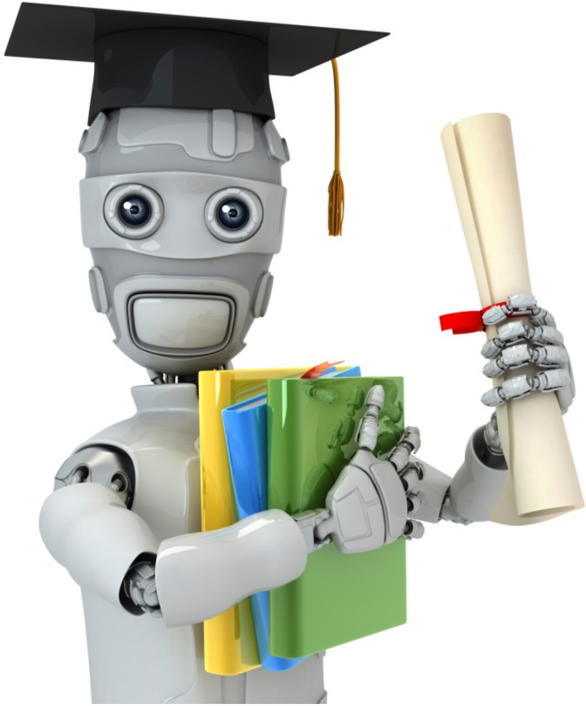
$x \rightarrow \underline{y}$

$x_1, x_2, \ldots, x_n$

PCA is not linear regression







Machine Learning

Dimensionality Reduction

Principal Component Analysis algorithm

Data preprocessing

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

Preprocessing (feature scaling/mean normalization):

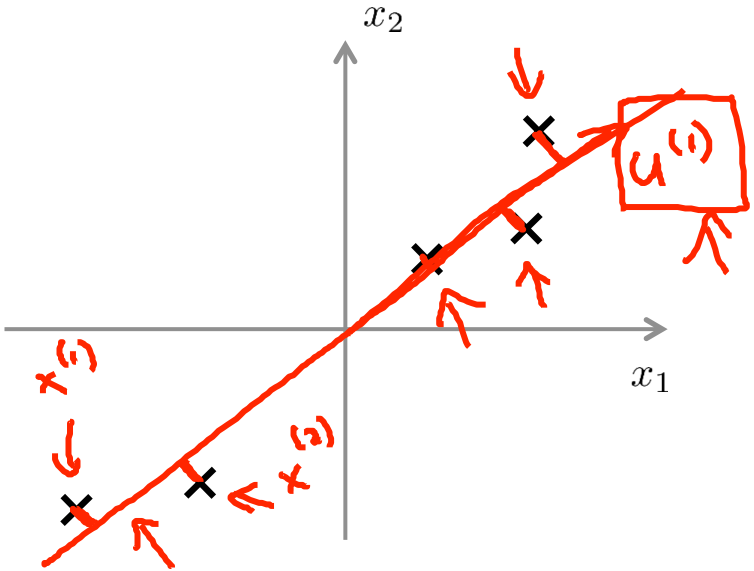
$$\mu_j = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)}$$

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.

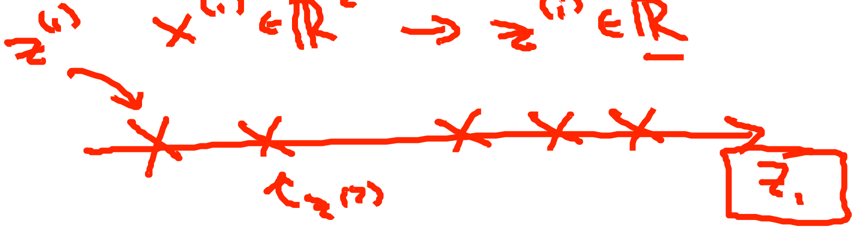
$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j}$$

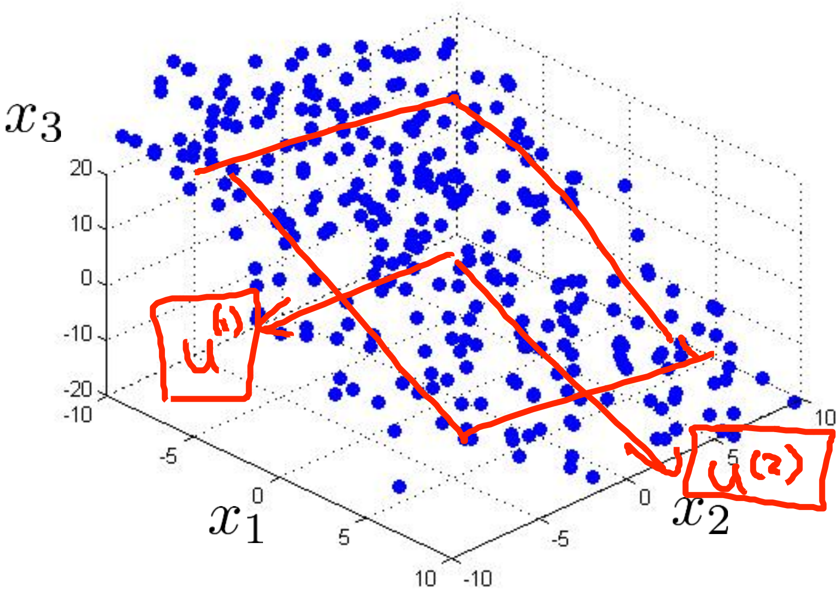
Principal Component Analysis (PCA) algorithm



Reduce data from 2D to 1D

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





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":

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

Sigma

Compute "eigenvectors" of matrix Σ :

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

n×n matrix.

→ Singular value decomposition

eig(Sigma)

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

$\underbrace{u^{(1)}\ u^{(2)}\ u^{(3)}}_{k}$

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

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

Principal Component Analysis (PCA) algorithm

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

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

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

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

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

U_{reduce}

Principal Component Analysis (PCA) algorithm summary

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

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

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

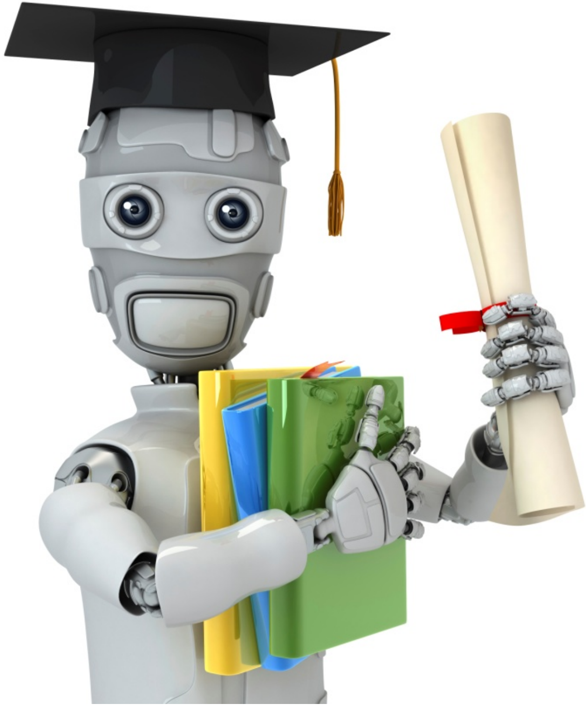
$\underline{X} = \begin{bmatrix} — & x^{(1)T} & — \\ & \vdots & \\ — & x^{(m)T} & — \end{bmatrix}$

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

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

$\cancel{x_0 = 1}$

Andrew Ng

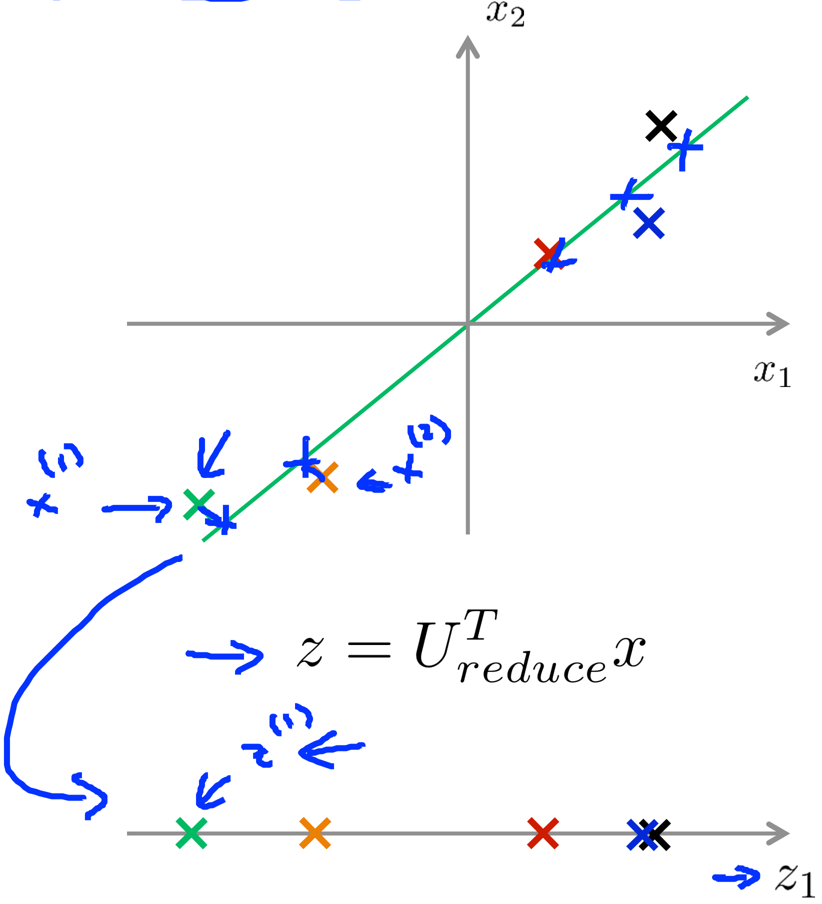


Machine Learning

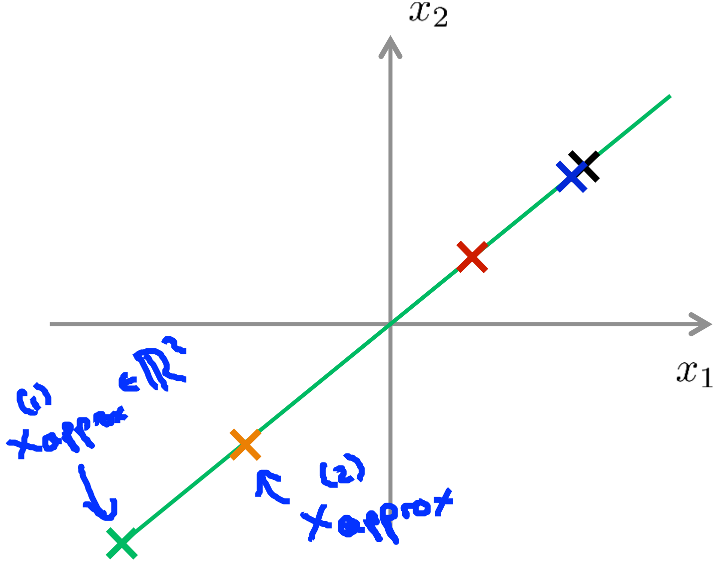
Dimensionality Reduction

Reconstruction from compressed representation

Reconstruction from compressed representation



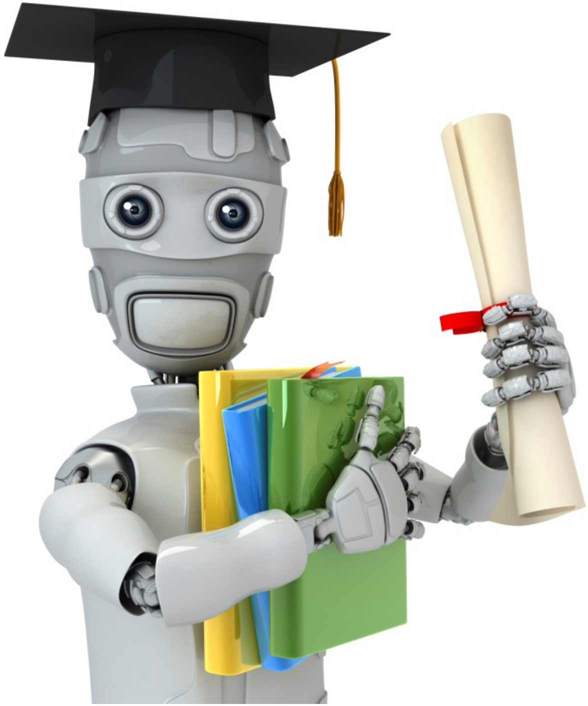
$$\rightarrow \quad z = U_{reduce}^T x$$



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

$$\overset{\tilde{x}}{\underset{\in \mathbb{R}^n}{x_{approx}^{(1)}}} = \underbrace{\underbrace{U_{reduce}}_{n \times k} \cdot \underbrace{z^{(1)}}_{k \times 1}}_{n \times 1}$$

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

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

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

0.10 (10%)

→ “~~99%~~ of variance is retained”

~~95%~~ 90%

Choosing k (number of principal components)

Algorithm:

Try PCA with ~~$k = 1$~~ ~~$k=2$~~ ~~$k=3$~~ $k=4$ ⋮

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

Check if

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

$k = 17$

```
→ [U,S,V] = svd(Sigma)
```

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

$k=3$

For given k

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

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

Andrew Ng

Choosing k (number of principal components)

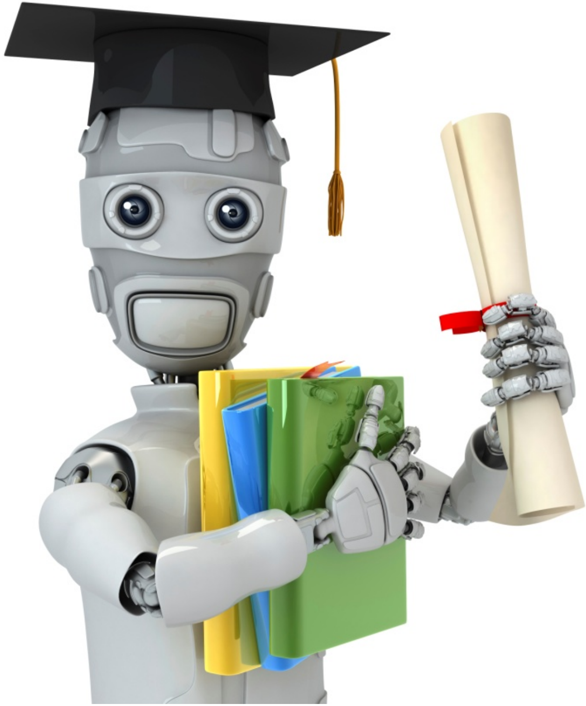
```
[U,S,V] = svd(Sigma)
```

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)



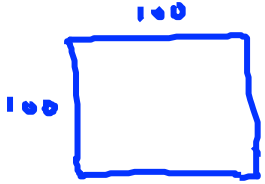
Machine Learning

Dimensionality Reduction

Advice for applying PCA

Supervised learning speedup

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



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

Extract inputs:

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

$$\downarrow PCA$$

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

$x \downarrow z$

$\underline{U_{reduce}}$

New training set:

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

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

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.

$\underline{x \rightarrow z}$

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 $\underline{z^{(i)}}$ instead of $\underline{x^{(i)}}$ to reduce the number of features to $\overset{1000}{\underline{k}} < \underline{n}$. — 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.

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

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 $\underline{z^{(i)}}$.