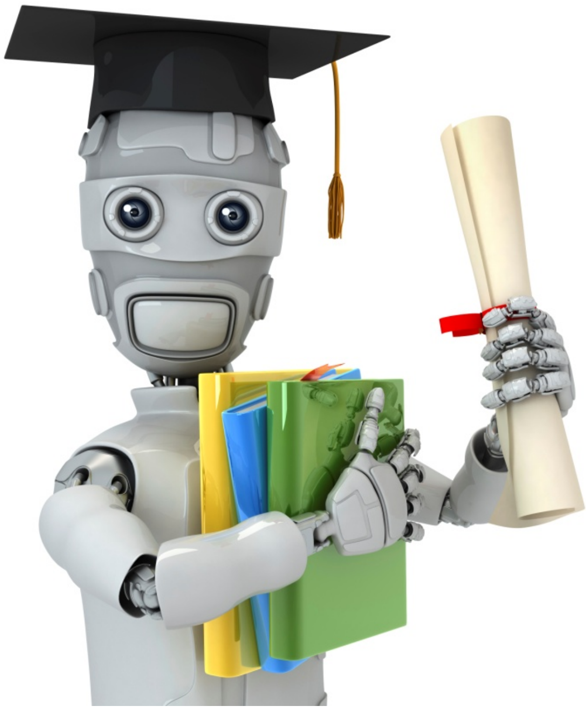
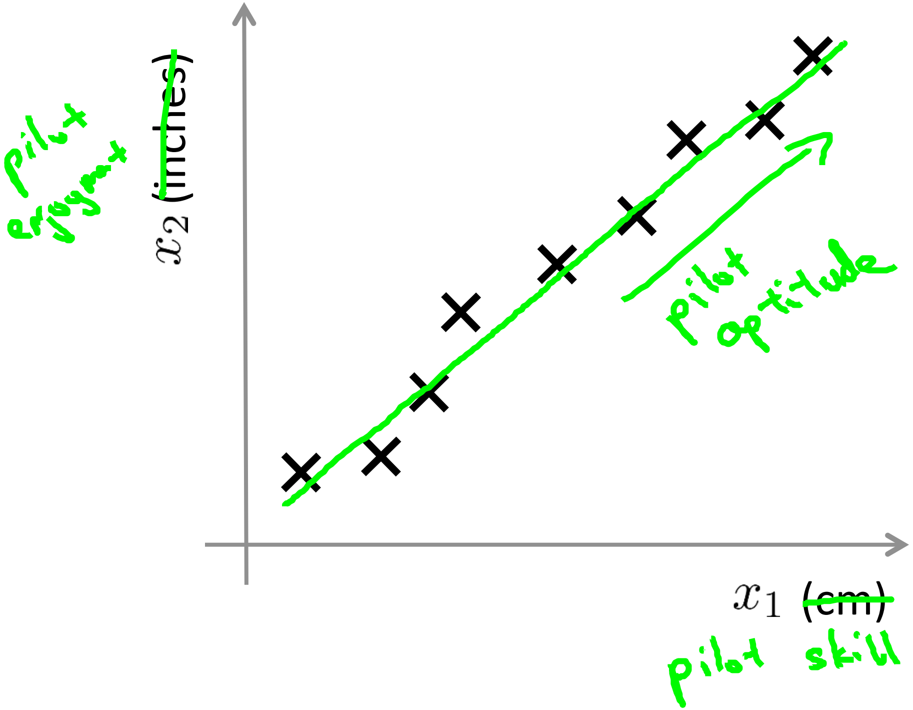


Machine Learning

Dimensionality Reduction

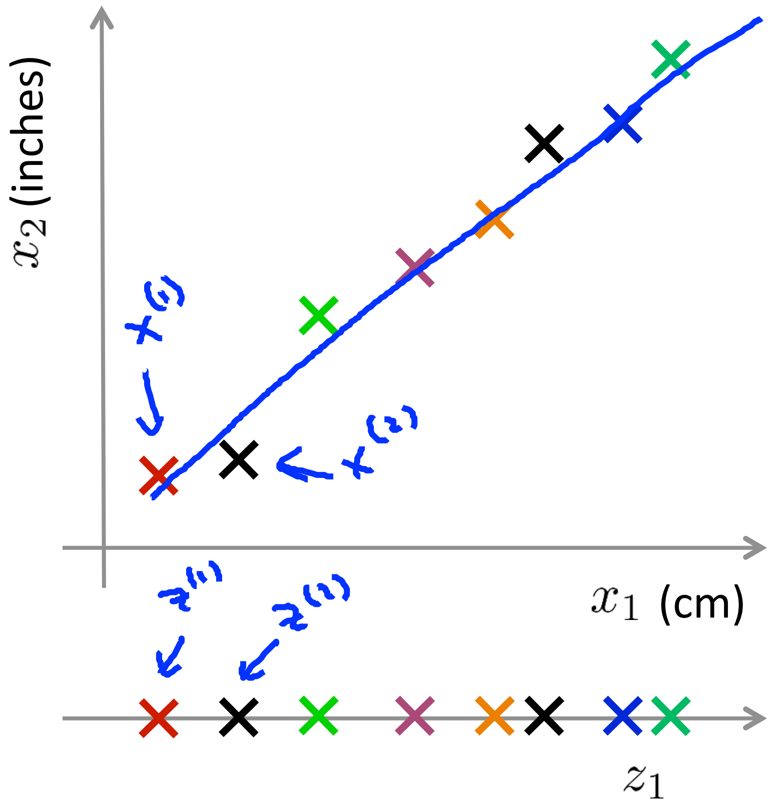
Motivation I: Data Compression

Data Compression



Reduce data from 2D to 1D

Data Compression



Reduce data from 2D to 1D

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

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

$$\vdots$$

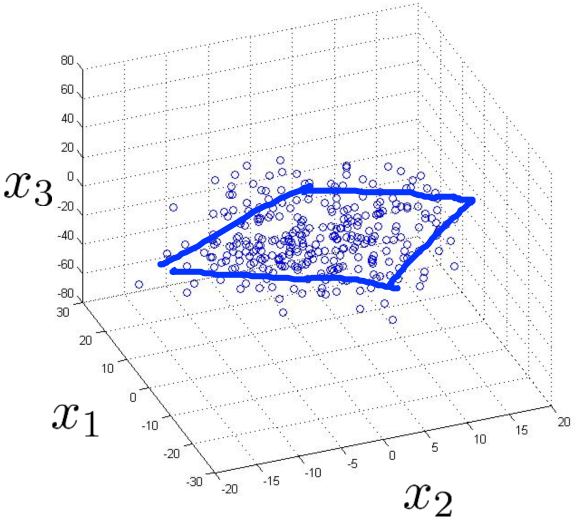
$$x^{(m)} \in \mathbb{R}^2 \rightarrow z^{(m)} \in \mathbb{R}$$

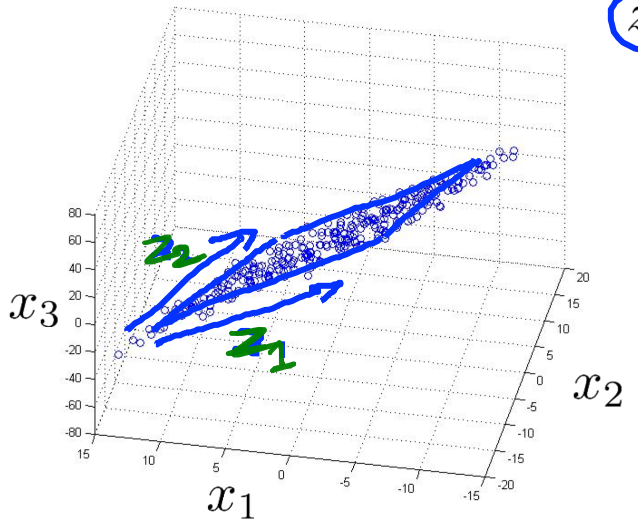
2-Dimension 1-Dimension

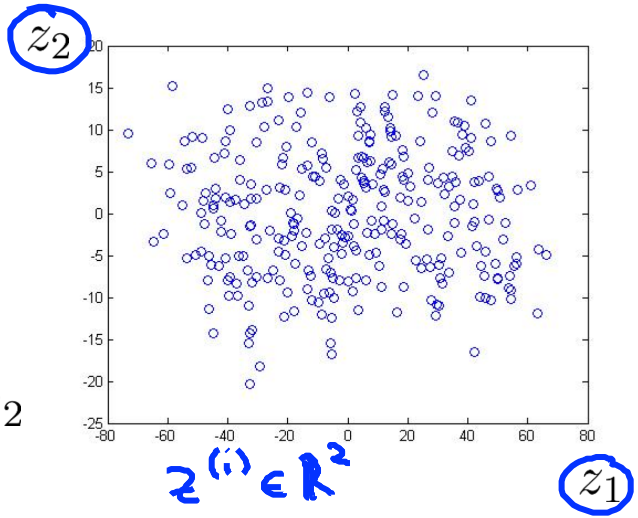
Data Compression

1000D → 100D

Reduce data from 3D to 2D





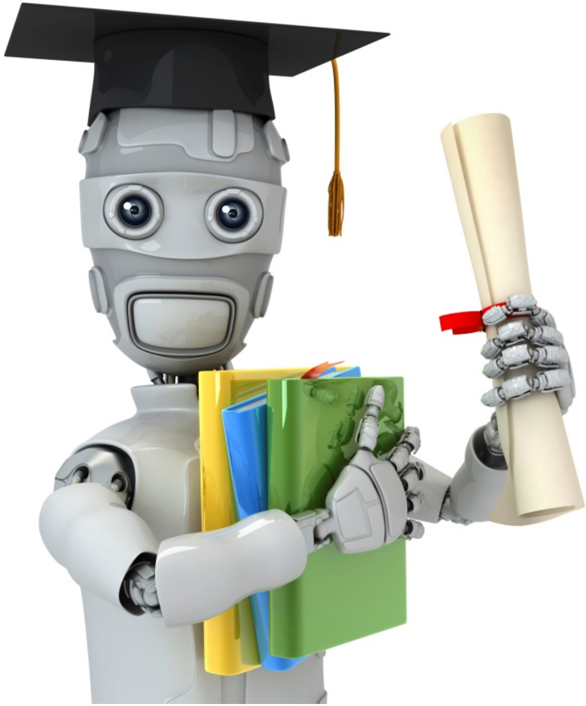


$x^{(i)} \in \mathbb{R}^3$

3-D points

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

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



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]

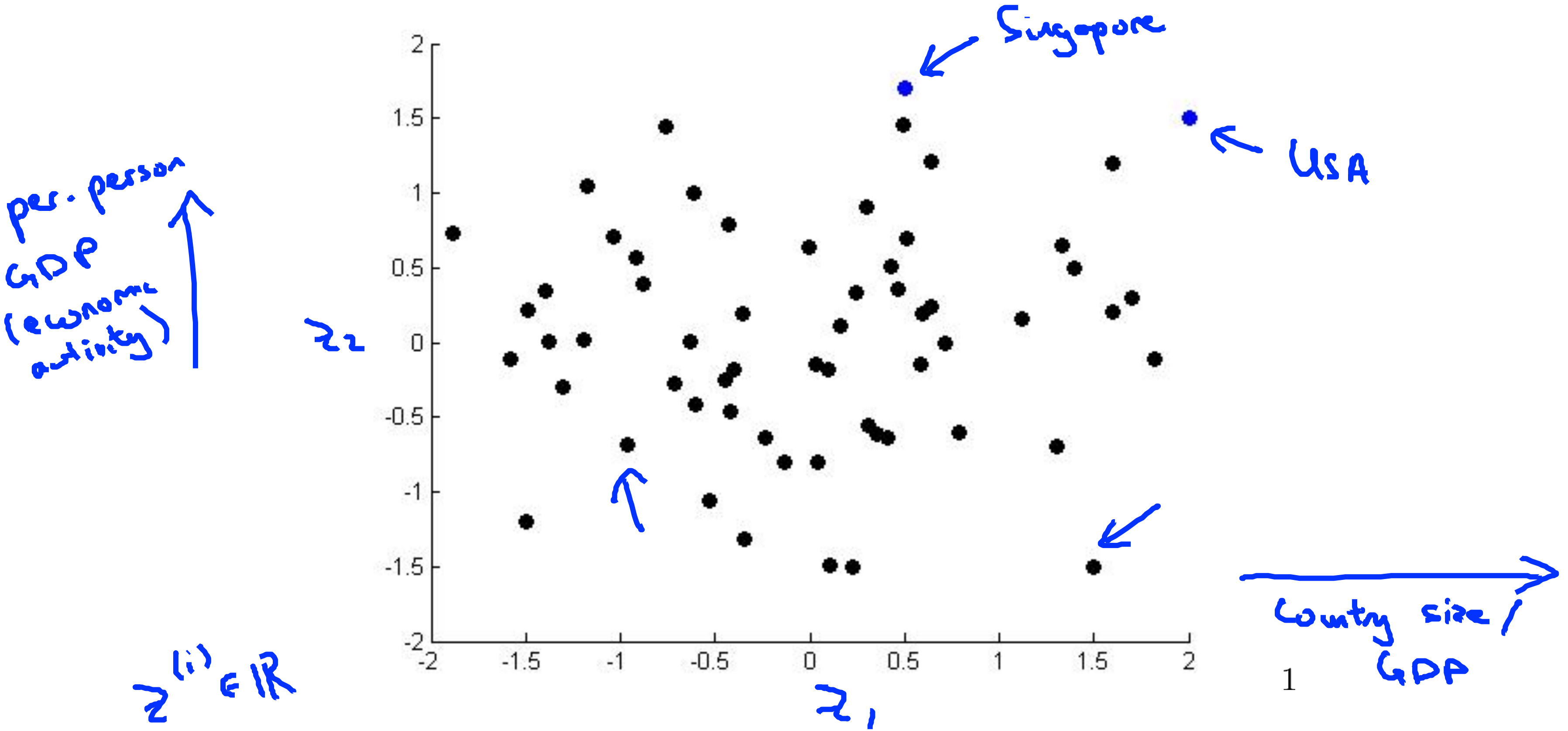
Data Visualization

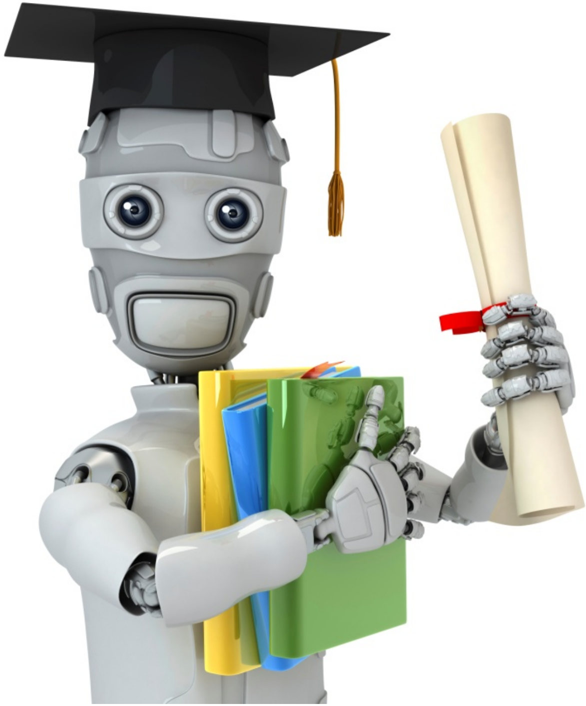
Country	z_1	z_2
Canada	1.6	1.2
China	1.7	0.3
India	1.6	0.2
Russia	1.4	0.5
Singapore	0.5	1.7
USA	2	1.5
…	…	…

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

Reduce data from 50D to 2D

Data Visualization



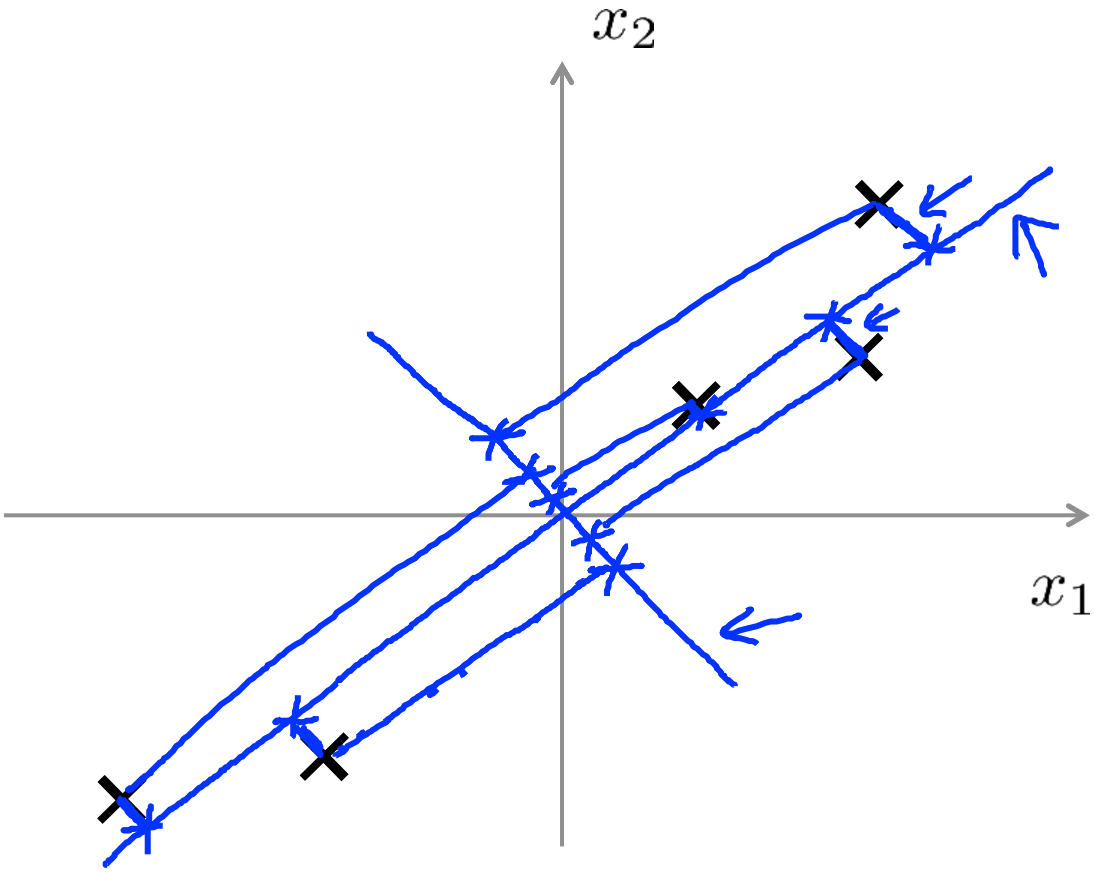


Machine Learning

Dimensionality Reduction

Principal Component Analysis problem formulation

Principal Component Analysis (PCA) problem formulation

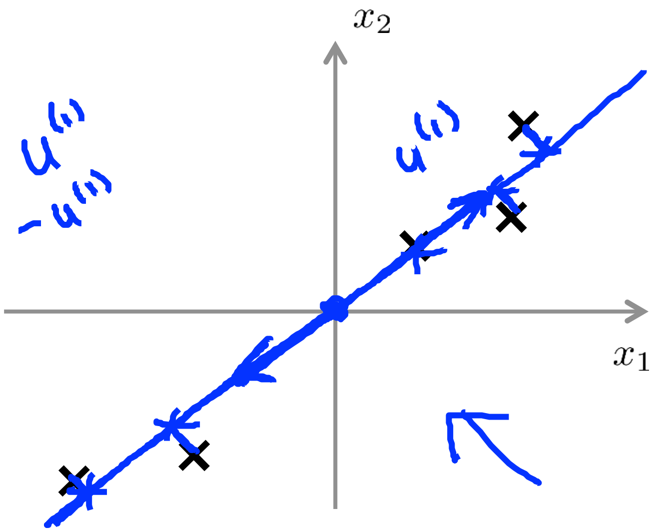


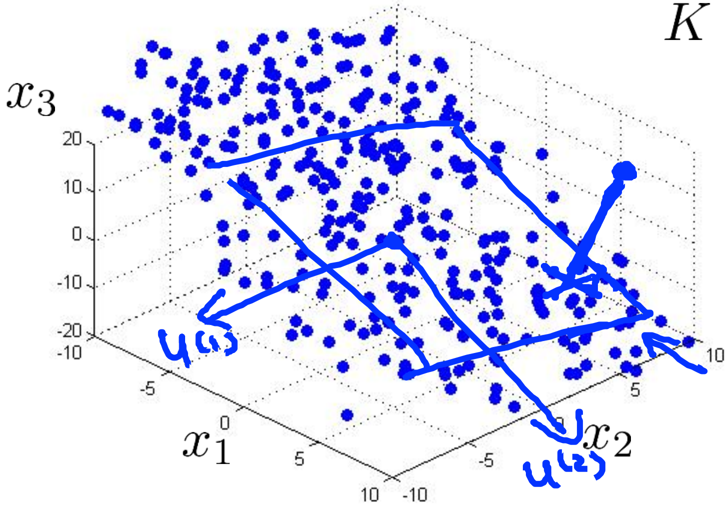
$x \in \mathbb{R}^2$

Principal Component Analysis (PCA) problem formulation

$3D \rightarrow 2D$

$K = 2$

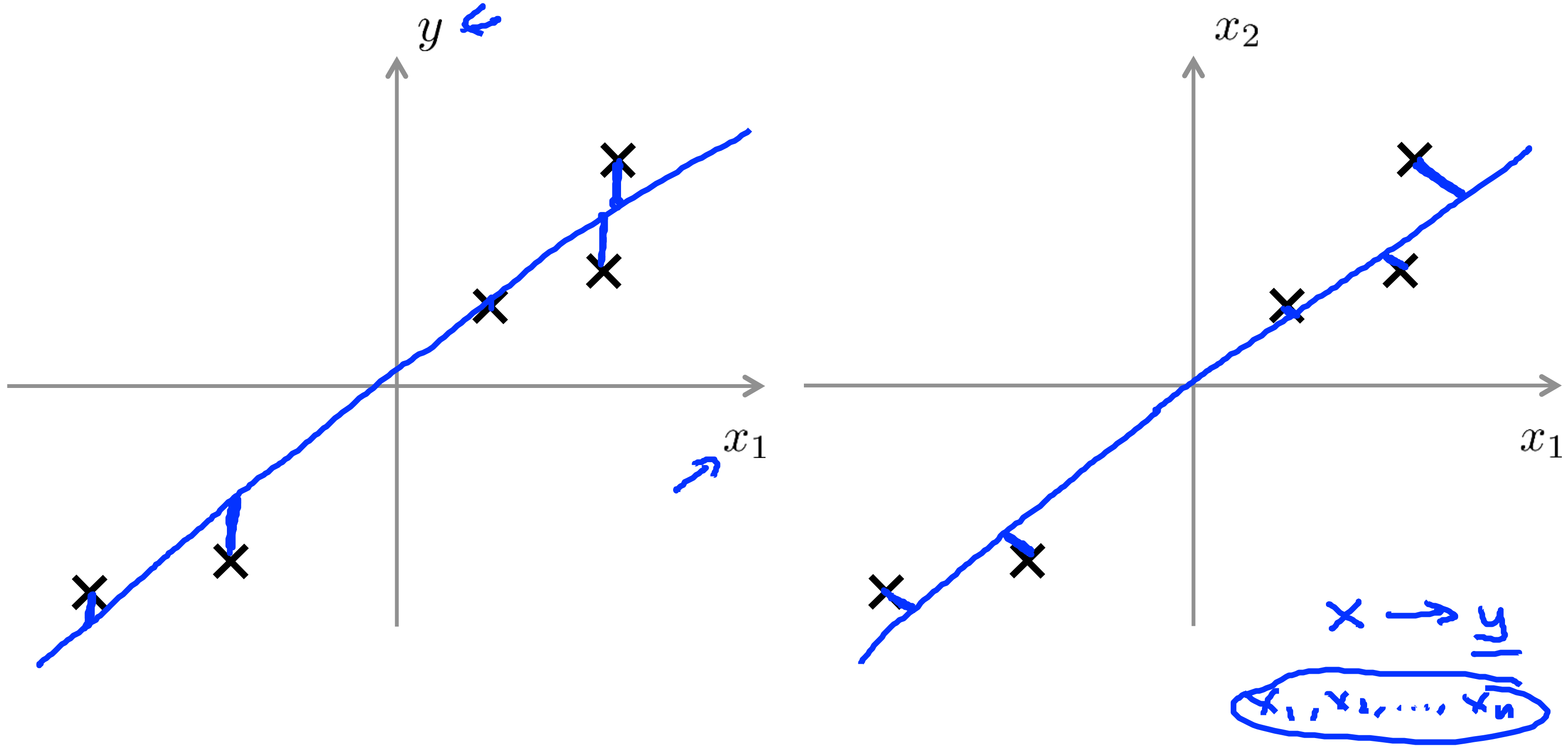




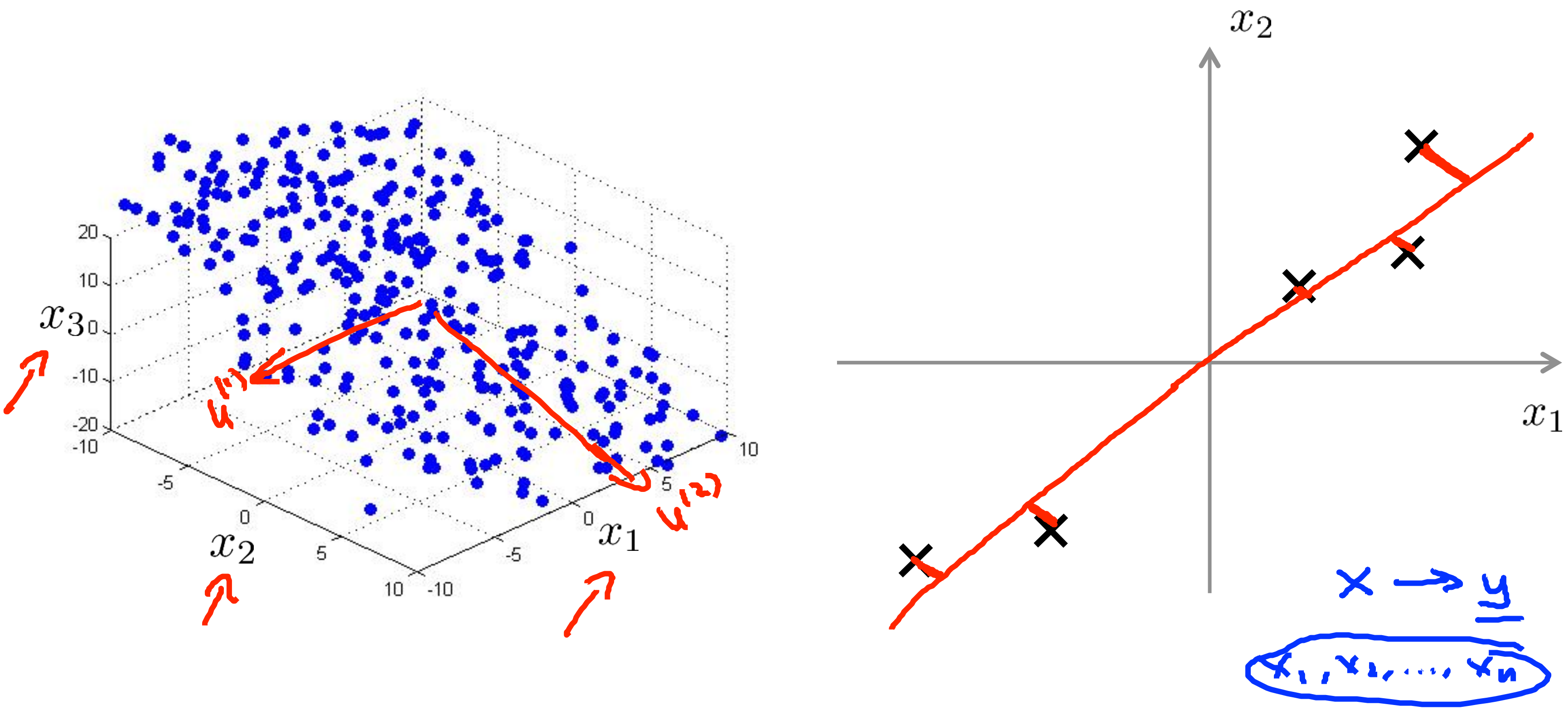
Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

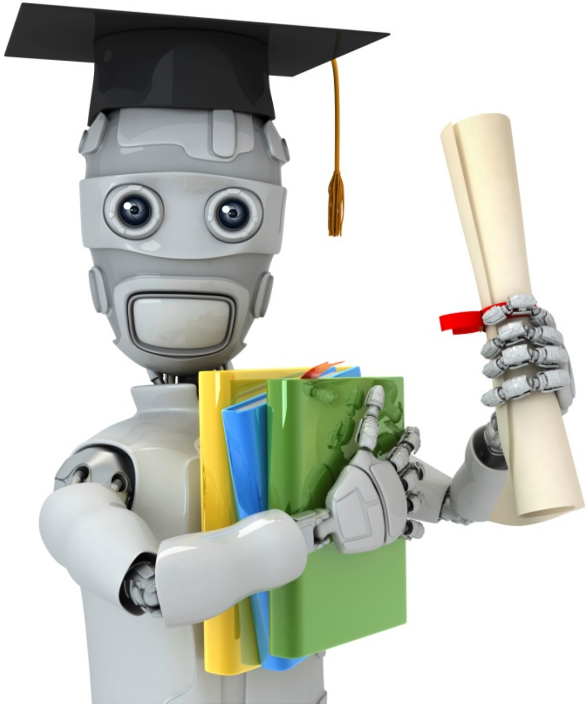
Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

PCA is not linear regression



PCA is not linear regression





Machine Learning

Dimensionality Reduction

Principal Component Analysis algorithm

Data preprocessing

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

Preprocessing (feature scaling/mean normalization):

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

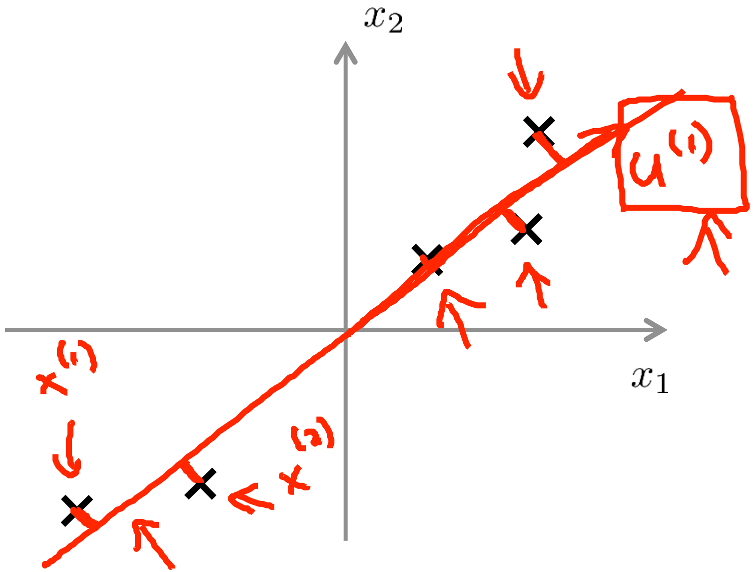
Replace each $x_j^{(i)}$ with $x_j - \mu_j$.

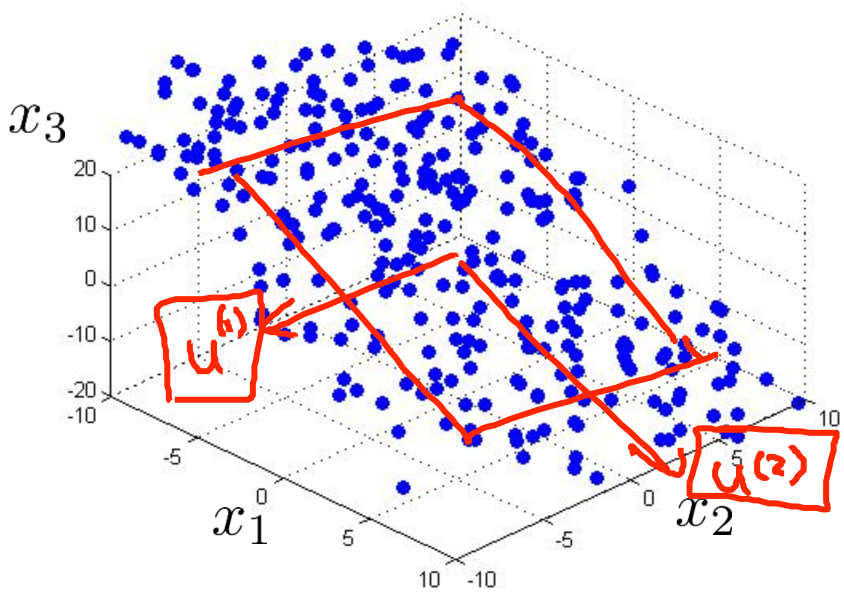
If different features on different scales (e.g., $x_1 =$ size of house, $x_2 =$ number of bedrooms), scale features to have comparable range of values.

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

Andrew Ng

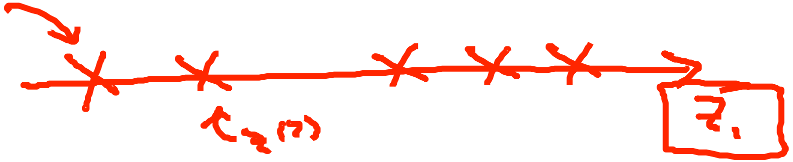
Principal Component Analysis (PCA) algorithm





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":

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

n×n

Sigma

Compute "eigenvectors" of matrix Σ :

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

→ Singular value decomposition

eig(Sigma)

n×n matrix.

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

k

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

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

Andrew Ng

Principal Component Analysis (PCA) algorithm

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

$$\rightarrow U = \Bigg[\underbrace{\begin{matrix} | & | \\ u^{(1)} & u^{(2)} \\ | & | \end{matrix}}_{k} \;\; \cdots \;\; \begin{matrix} | \\ u^{(n)} \\ | \end{matrix}\Bigg] \in \mathbb{R}^{n\times n}$$

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

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

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

Principal Component Analysis (PCA) algorithm summary

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

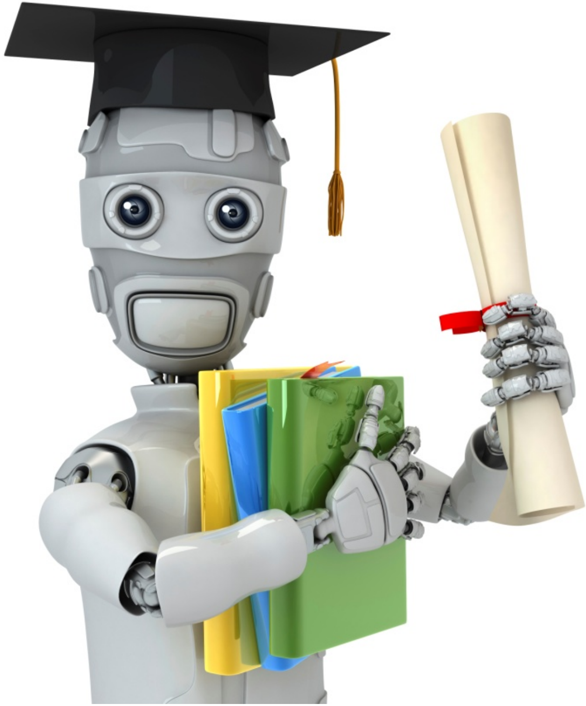
$$\text{Sigma} = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)})(x^{(i)})^T$$

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

Sigma = (1/m) * X' * X;

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

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

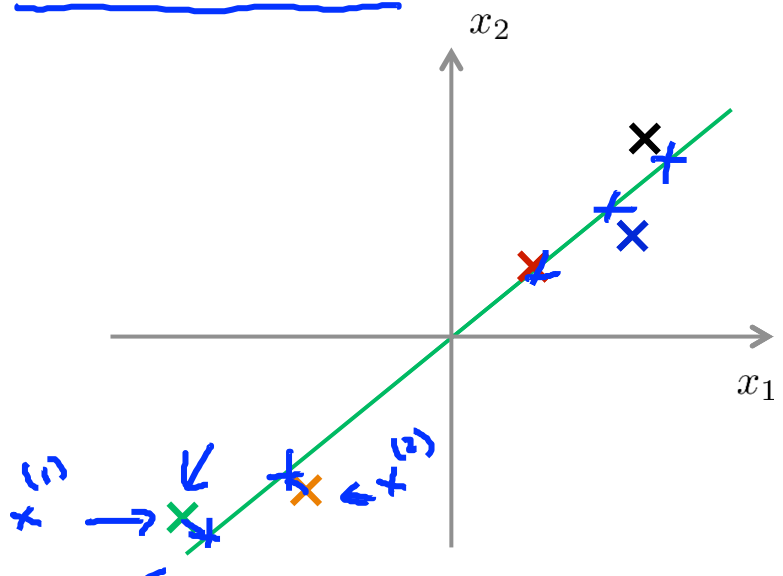


Machine Learning

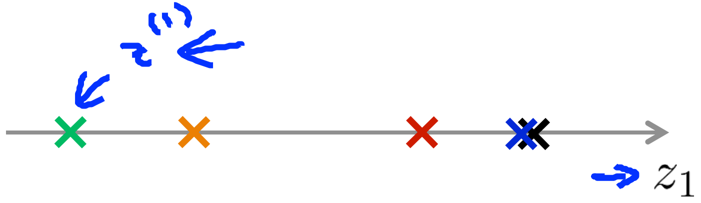
Dimensionality Reduction

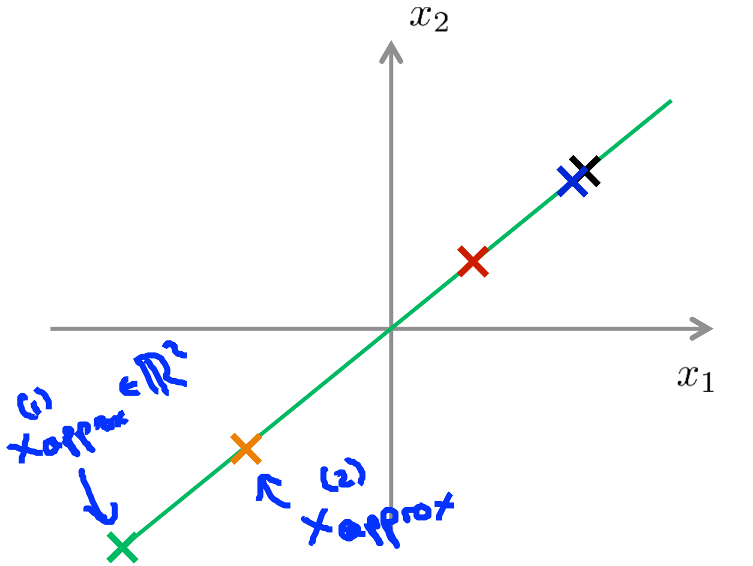
Reconstruction from compressed representation

Reconstruction from compressed representation



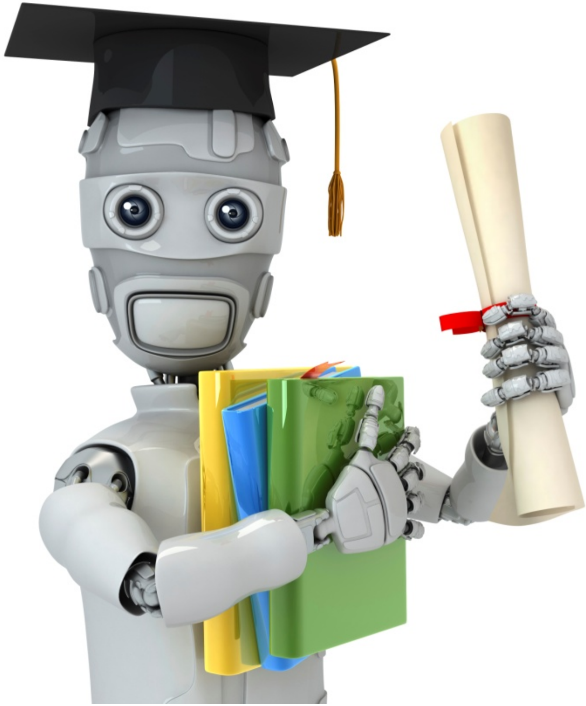
$$\rightarrow \quad z = U_{reduce}^T x$$





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

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



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

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

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

0.10 (10%)

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

~~95%~~ 90%

Choosing k (number of principal components)

Algorithm:

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

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

Check if

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

$k=17$

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

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

$k=3$

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)

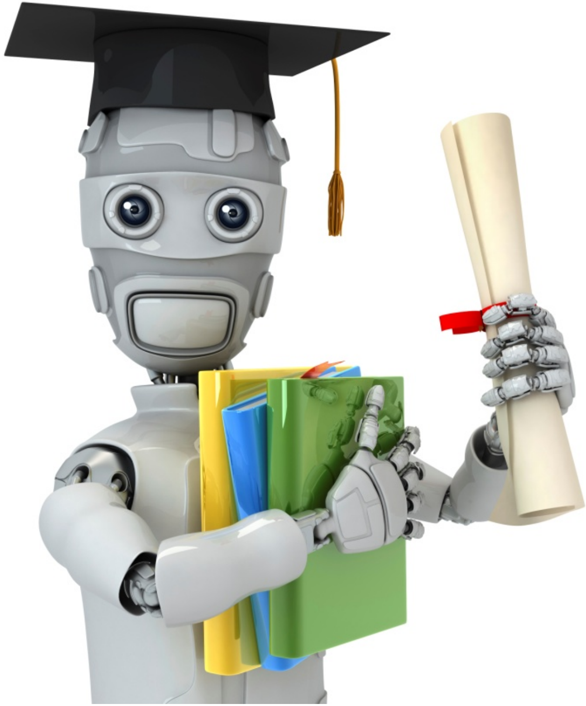
```
[U,S,V] = svd(Sigma)
```

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)

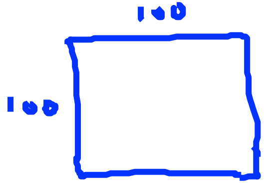


Machine Learning

Dimensionality Reduction

Advice for applying PCA

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



Supervised learning speedup

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

Extract inputs:

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

$\downarrow PCA$

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

$x \downarrow z$

U_{reduce}

New training set:

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

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

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.

$x \to z$

Andrew Ng

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 $k < n$.

1000

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