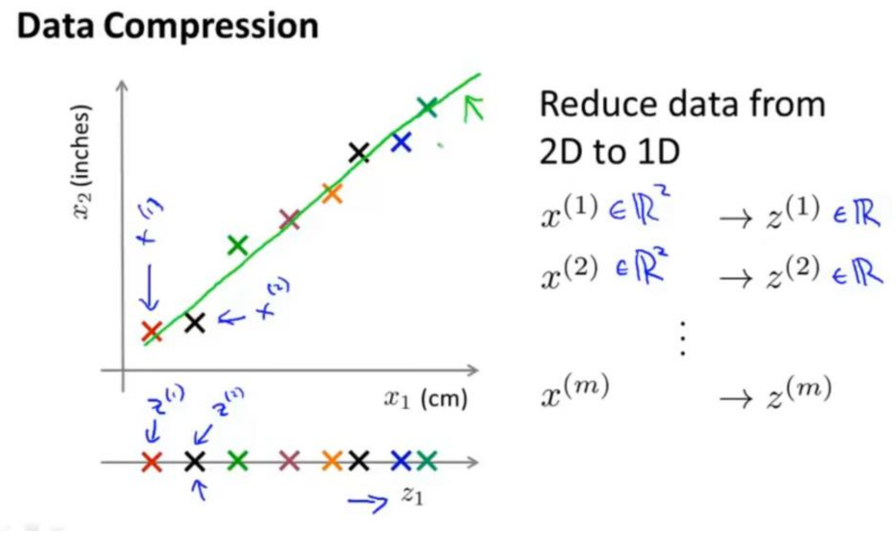
Dimensionality Reduction

1 Motivation I: Data Compression



Data Compression

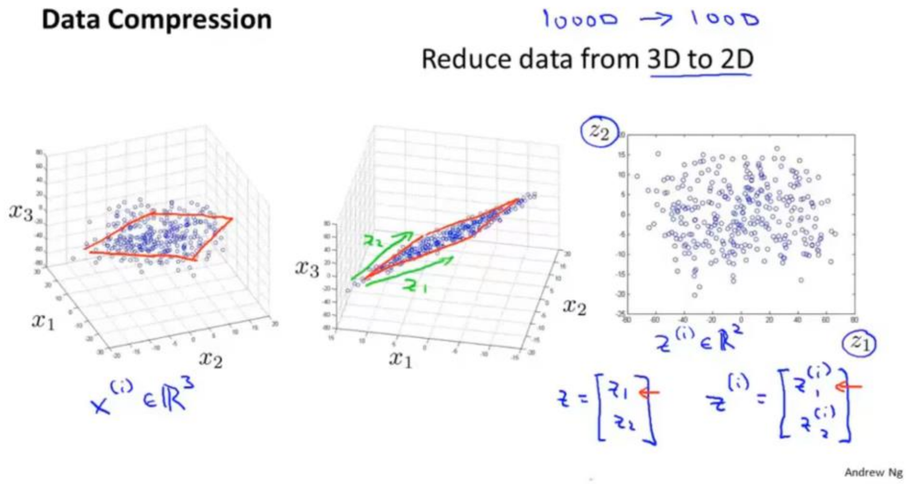
Reduce data from 2D to 1D

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

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

$\vdots$

$x^{(m)} \rightarrow z^{(m)}$



Data Compression

10000 → 1000

Reduce data from 3D to 2D

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

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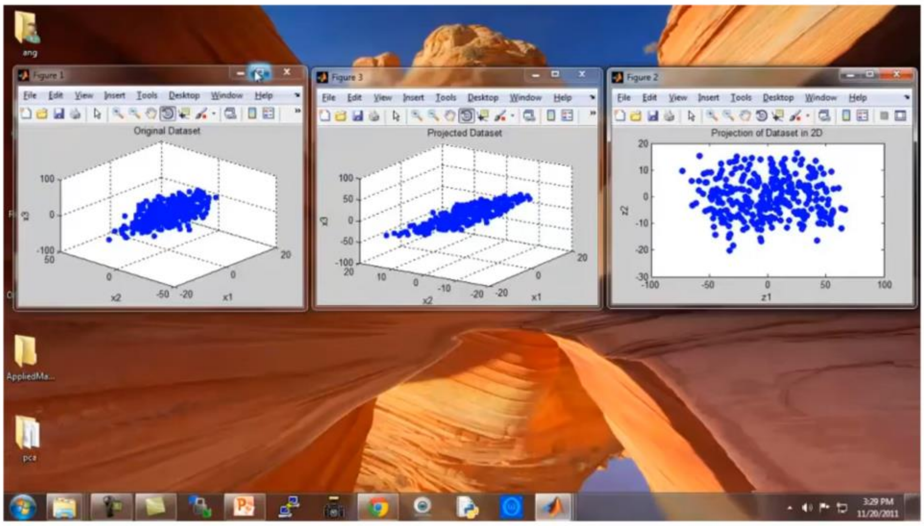
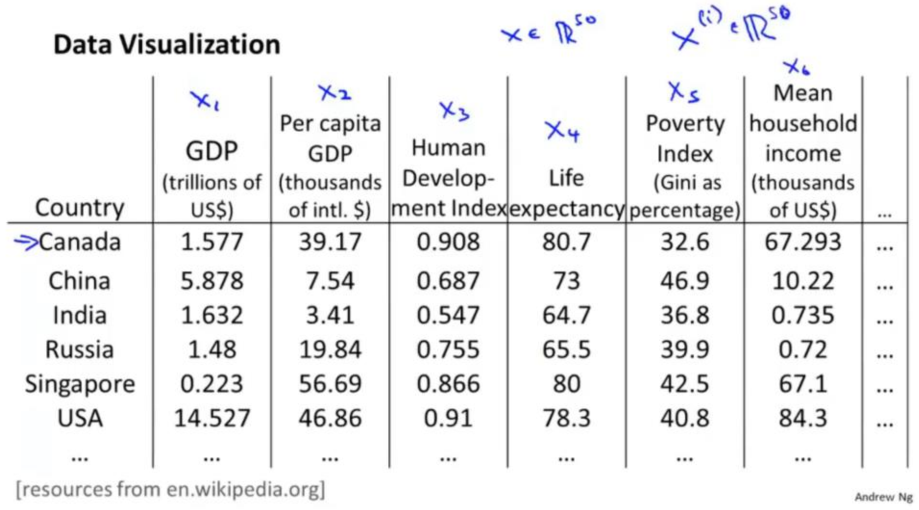


2 Motivation II: Data Visualization



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. $)	x_3 Human Development Index	x_4 Life expectancy	x_5 Poverty Index (Gini as percentage)	x_6 Mean household income (thousands of US$)	…
→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]

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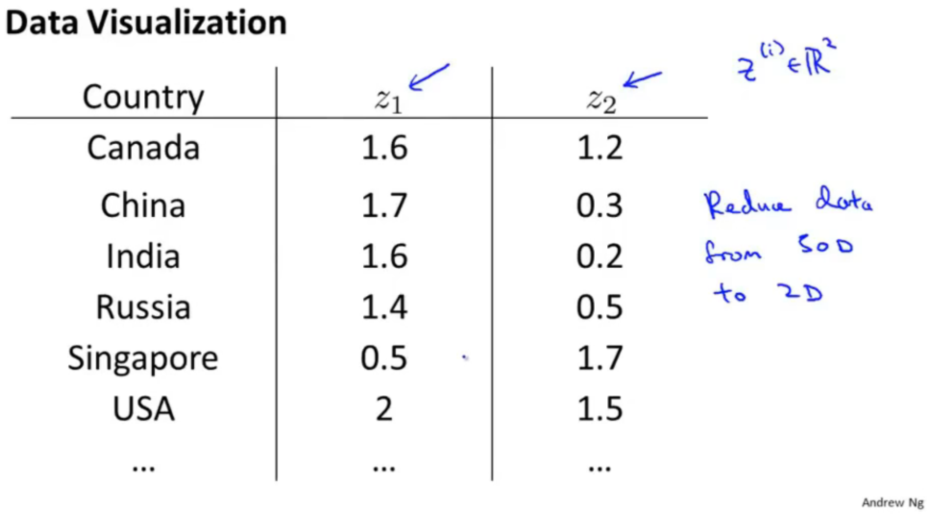

Data Visualization

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

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

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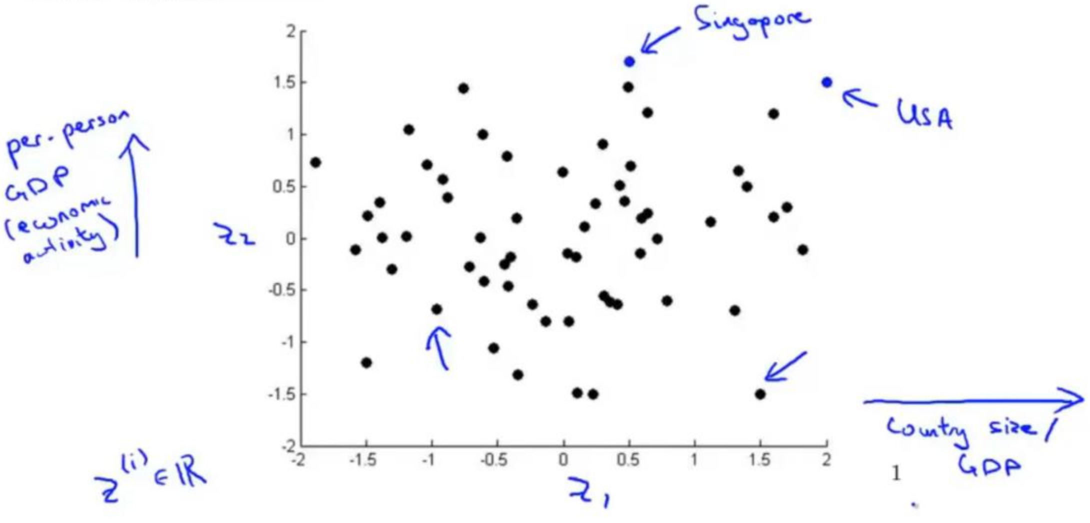
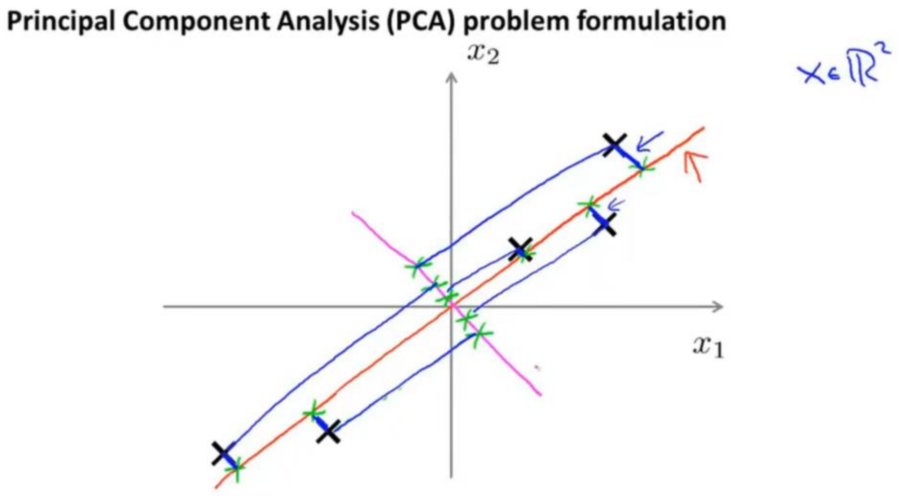
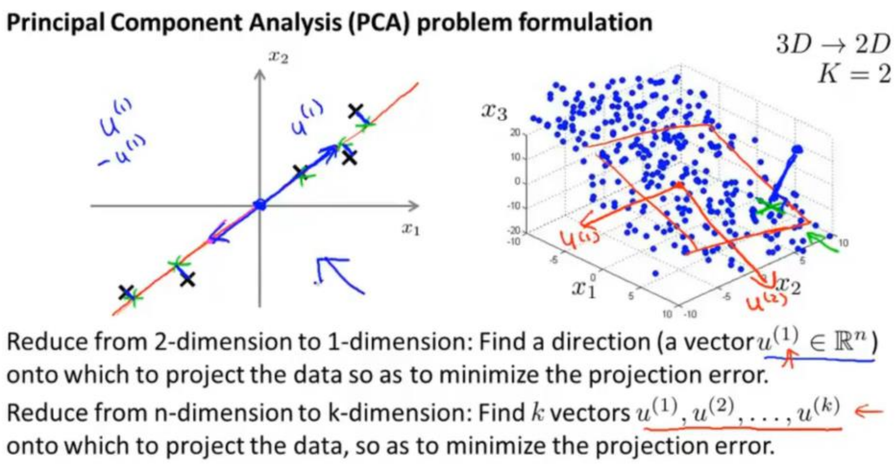
Data Visualization



3 Principal Component Analysis problem formulation



Principal Component Analysis (PCA) problem formulation

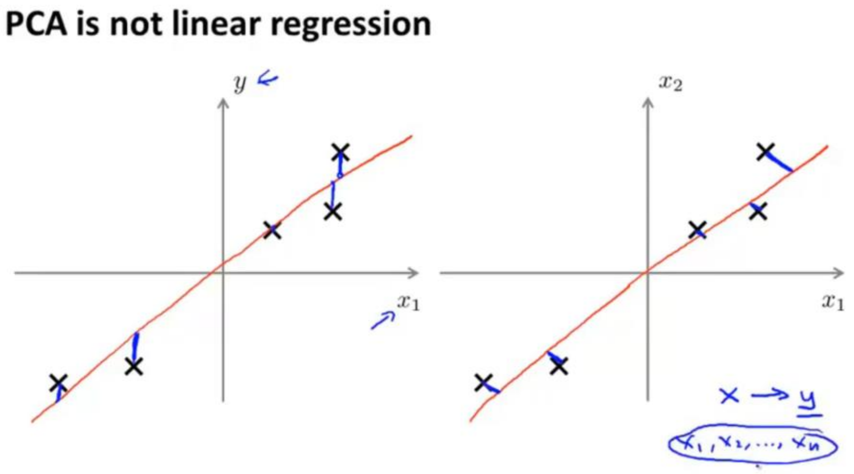


Principal Component Analysis (PCA) problem formulation

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

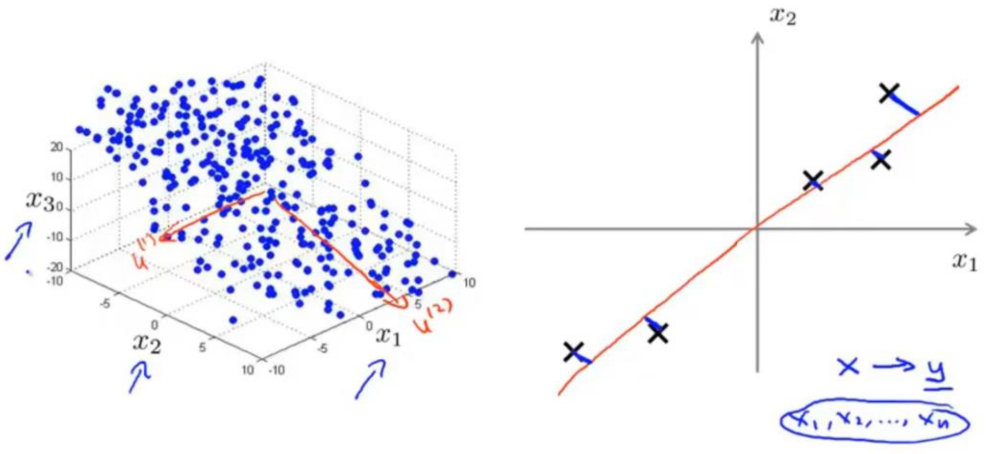
Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

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



4 Principal Component Analysis algorithm

Data preprocessing

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

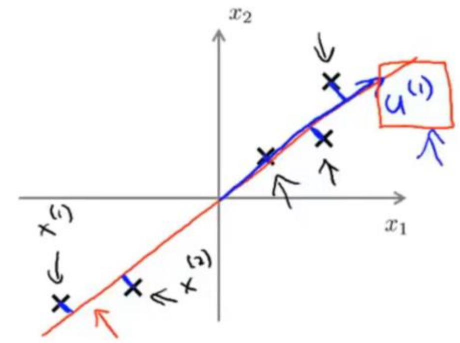
Preprocessing (feature scaling/mean normalization):

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

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

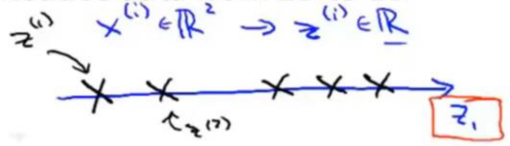
If different features on different scales (e.g., x_1 = size of house, x_2 = number of bedrooms), scale features to have comparable range of values.

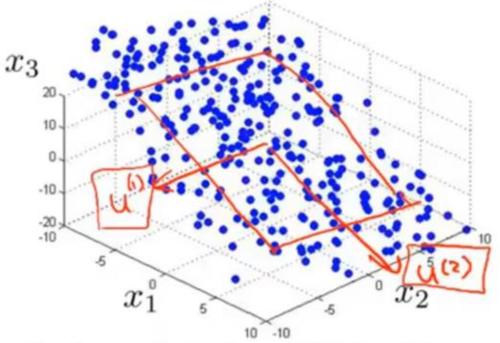
Principal Component Analysis (PCA) algorithm



Reduce data from 2D to 1D

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





Reduce data from 3D to 2D

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

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

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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.

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

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:

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

k

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

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

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

Ureduce

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Principal Component Analysis (PCA) algorithm summary

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

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

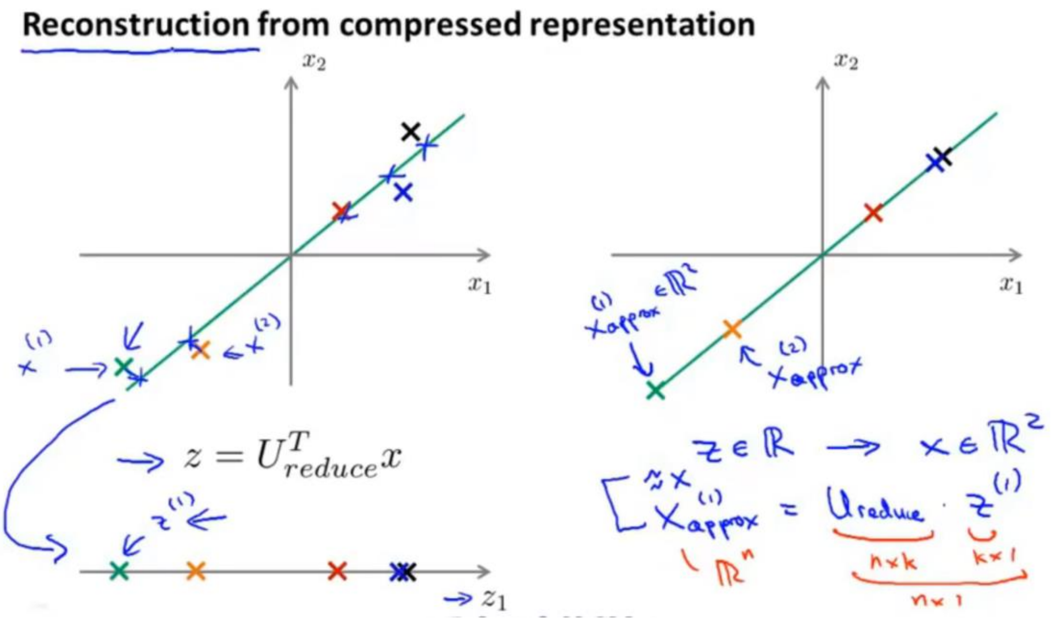
$$X = \begin{bmatrix} — x^{(1)T} — \\ \vdots \\ — x^{(m)T} — \end{bmatrix}$$

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

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

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

5 Reconstruction from compressed representation



Reconstruction from compressed representation

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

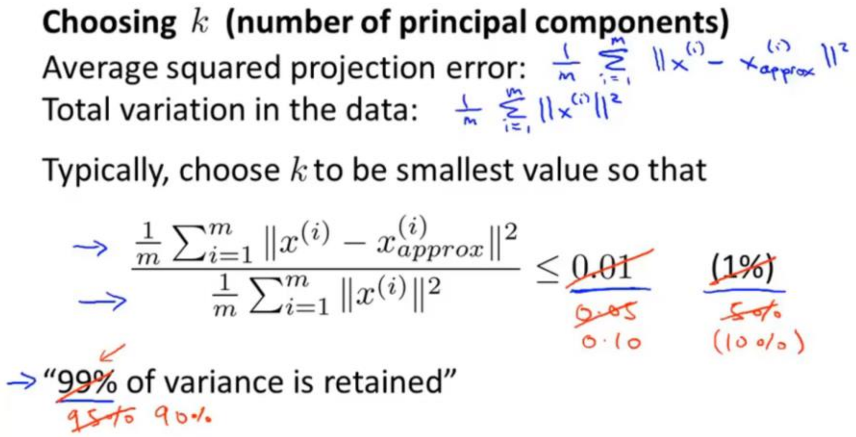
$z \in \mathbb{R} \rightarrow x \in \mathbb{R}^2$

$\approx x$

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

$\in \mathbb{R}^n$

6 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

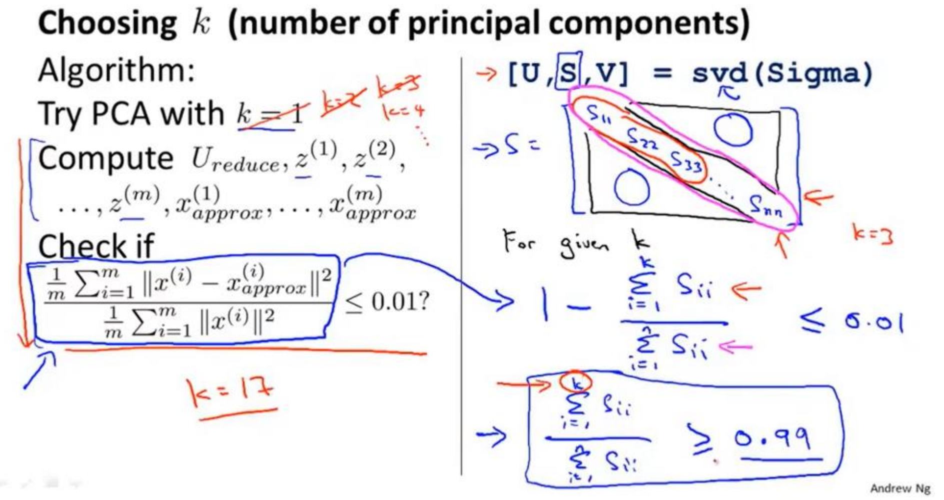
$$\rightarrow \frac{\frac{1}{m}\sum_{i=1}^{m} \|x^{(i)} - x_{approx}^{(i)}\|^2}{\frac{1}{m}\sum_{i=1}^{m} \|x^{(i)}\|^2} \leq \cancel{0.01} \quad (\cancel{1\%})$$

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

0.10 (10%)

→ "~~99%~~ of variance is retained"

~~95%~~ 90%



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

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

k=17

→ `[U,S,V] = svd(Sigma)`

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

k=3

For given k

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

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

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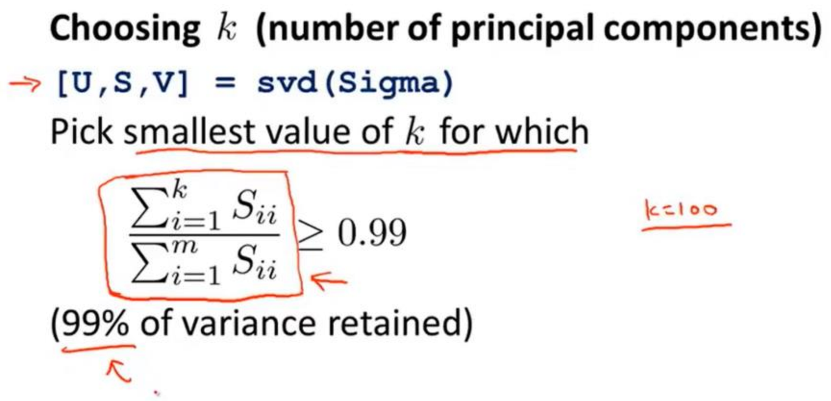


Choosing k (number of principal components)

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

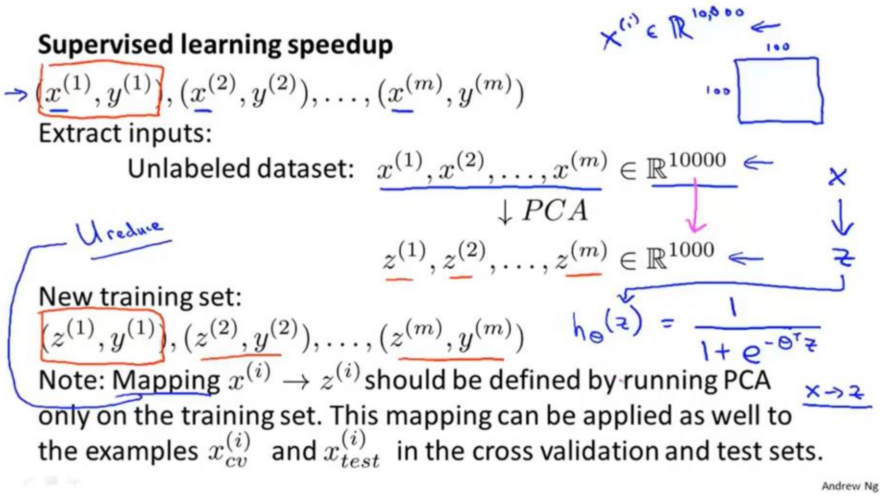
Pick smallest value of k for which

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

(99% of variance retained)

k=100

7 Advice for applying PCA



Supervised learning speedup

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

Extract inputs:

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

$\downarrow PCA$

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

New training set:

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

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.

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

100

100

$x \rightarrow z$

U_{reduce}

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

$x \rightarrow z$

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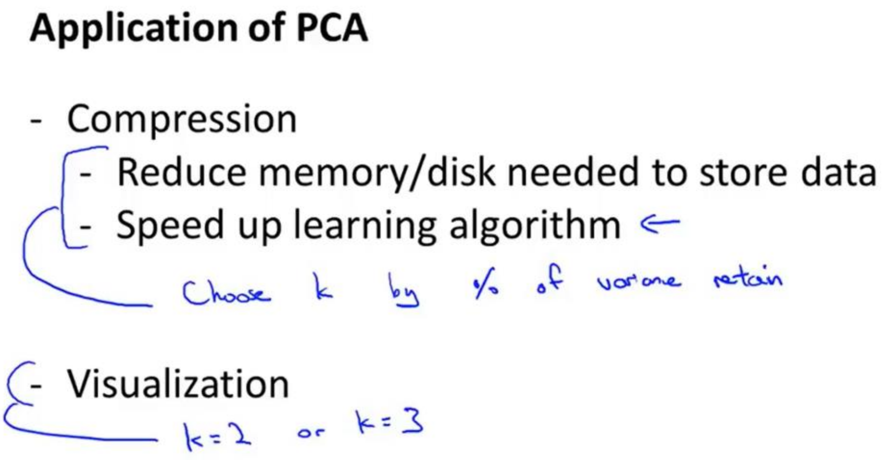

Application of PCA

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