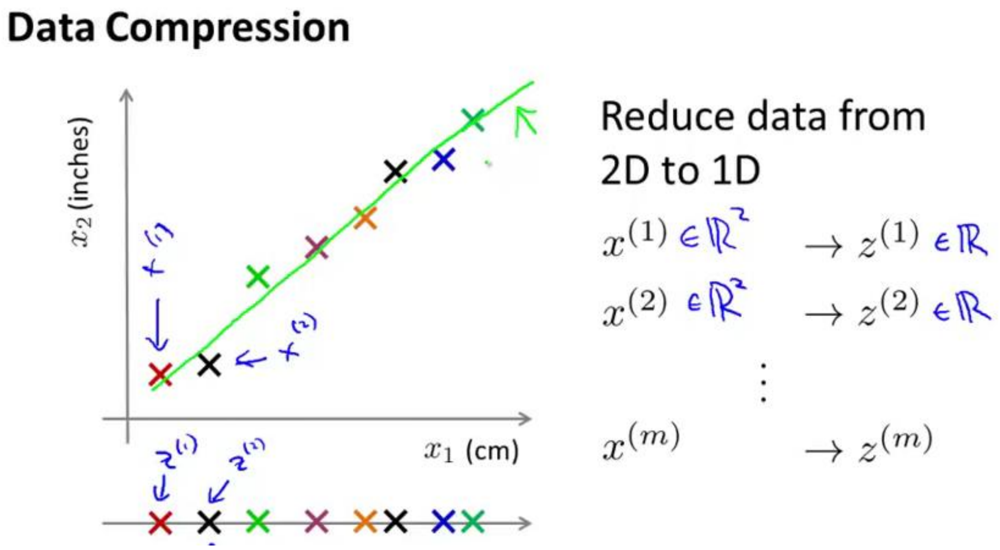
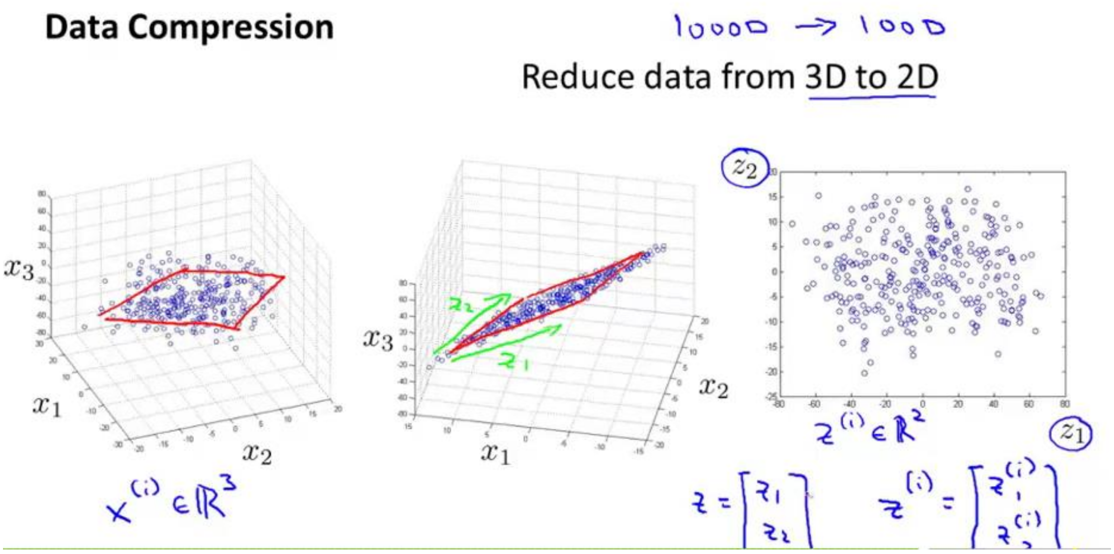
维数约减





数据可视化　降维

Data Visualization

$x \in \mathbb{R}^{50}$

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	...

Data Visualization

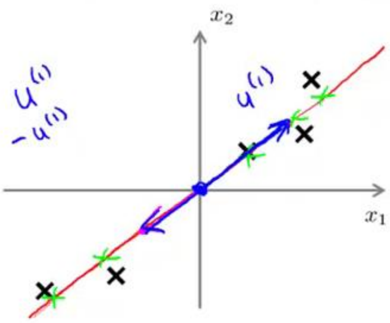
$z^{(i)} \in$

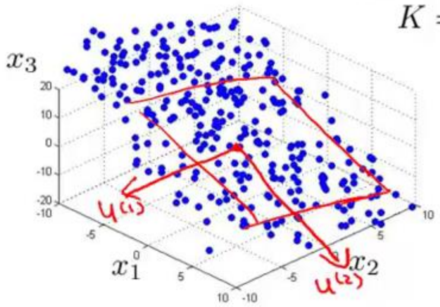
Country	z_1	z_2
Canada	1.6	1.2
China	1.7	0.3
India	1.6	0.2
Russia	1.4	0.5
Singapore	0.5	1.7
USA	2	1.5

主城分分析法　Principal Componet Analysis PCA

Principal Component Analysis (PCA) problem formulation

$3D \to 2D$
$K = 2$





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 实现

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.

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

协方差矩阵 covariance matrix

顺便说一下 svd 表示奇异值分解 (singular value decomposition)

Principal Component Analysis (PCA) algorithm

Reduce data from n-dimensions to k-dimensions

Compute "covariance matrix":

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

Compute "eigenvectors" of matrix Σ:

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

n×n matrix.

→ Singular value decomposition

eig (Sigma)

$$U = \begin{bmatrix} | & | & | & & | \\ u^{(1)} & u^{(2)} & u^{(3)} & \ldots & u^{(m)} \\ | & | & | & & | \end{bmatrix} \qquad U \in \mathbb{R}^{n\times n}$$

Principal Component Analysis (PCA) algorithm

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

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

k

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

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

U_{reduce}

Principal Component Analysis (PCA) algorithm summary

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

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

$$X = \left[\begin{array}{c} — x^{(1)T} — \\ \vdots \\ — x^{(m)T} — \end{array}\right]$$

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

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

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

减少

平均平方映射误差 (Average Squared Projection Error)

Choosing k (number of principal components)

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

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

Typically, choose k to be smallest value so that

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

~~0.05~~ ~~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 $U_{reduce}, z^{(1)}, z^{(2)}, \ldots, z^{(m)}, x^{(1)}_{approx}, \ldots, x^{(m)}_{approx}$

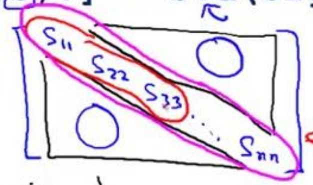
Check if

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

k=17

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

S =



k=3

For given k

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

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

99%的差异性被保留了下来

Choosing k (number of principal components)

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

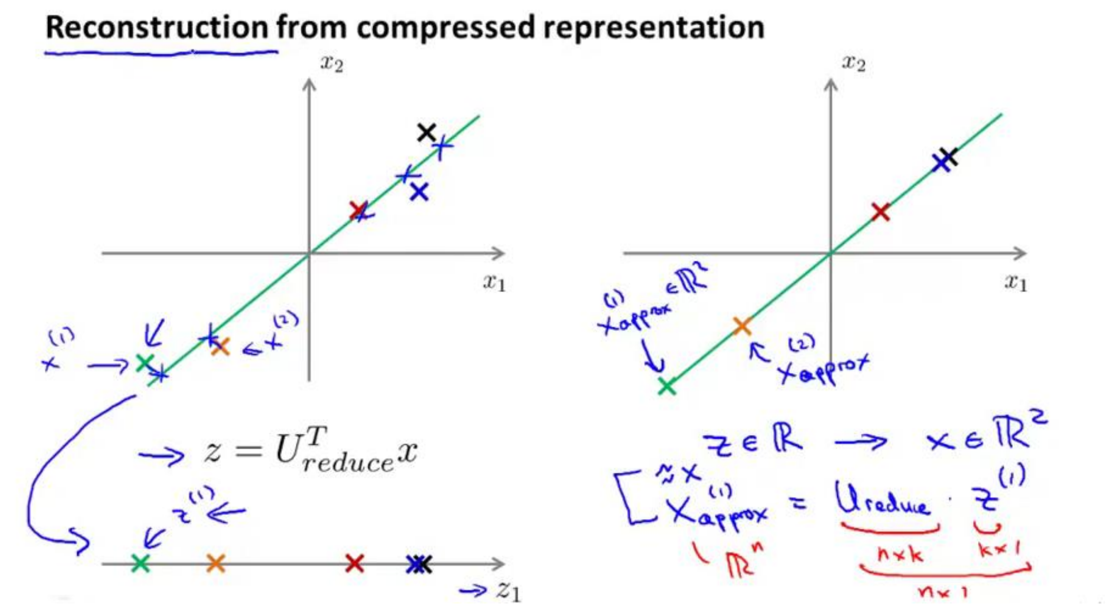
Pick smallest value of k for which

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

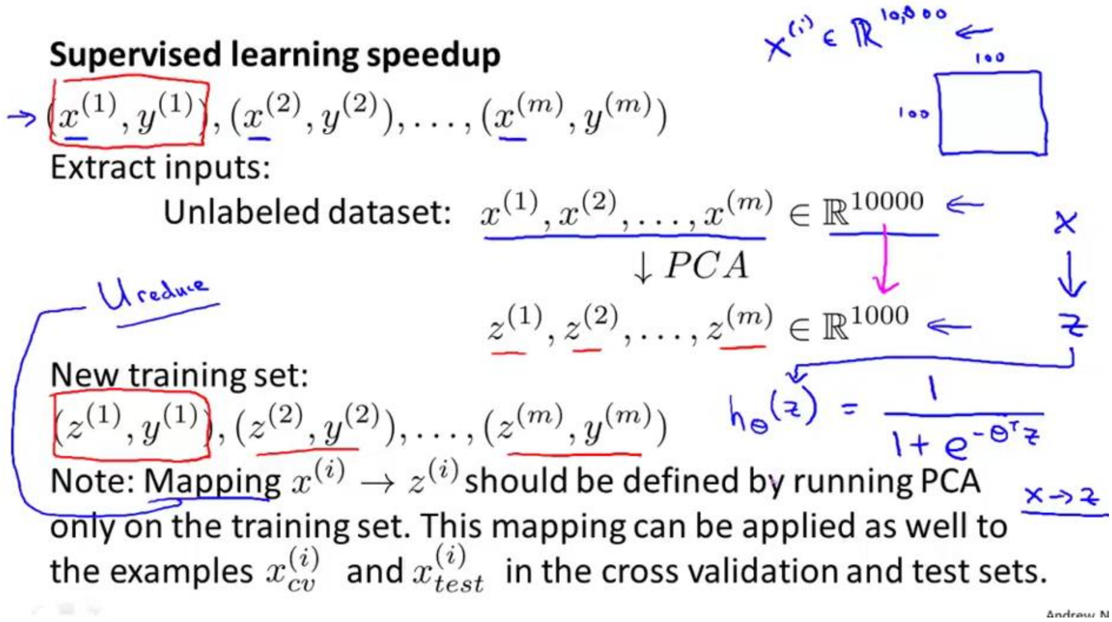
k=100

(99% of variance retained)

恢复减维



Reconstruction from compressed representation
x_2
x_1
$x^{(1)}$
$\in x^{(2)}$
$z = U_{reduce}^T x$
$z^{(1)}$
z_1
x_2
x_1
$x_{approx}^{(1)} \in \mathbb{R}^2$
$x_{approx}^{(2)}$
$z \in \mathbb{R} \rightarrow x \in \mathbb{R}^2$
$\approx x$
$x_{approx}^{(1)} = U_{reduce} \cdot z^{(1)}$
$\mathbb{R}^n$
$n \times k$
$k \times 1$
$n \times 1$



Supervised learning speedup
$x^{(i)} \in \mathbb{R}^{10,000}$
100
100
$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$
Extract inputs:
Unlabeled dataset: $x^{(1)}, x^{(2)}, \ldots, x^{(m)} \in \mathbb{R}^{10000}$
$\downarrow PCA$
$z^{(1)}, z^{(2)}, \ldots, z^{(m)} \in \mathbb{R}^{1000}$
$x \rightarrow z$
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.
$x \rightarrow z$
Andrew N

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 $z^{(i)}$.