Dimensionality Reduction

Machine Learning (AIM 5002-41)

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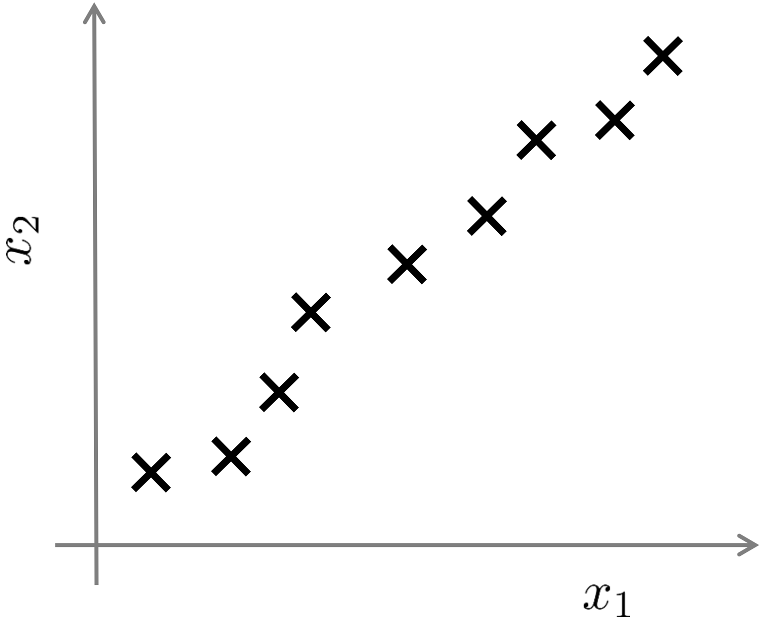
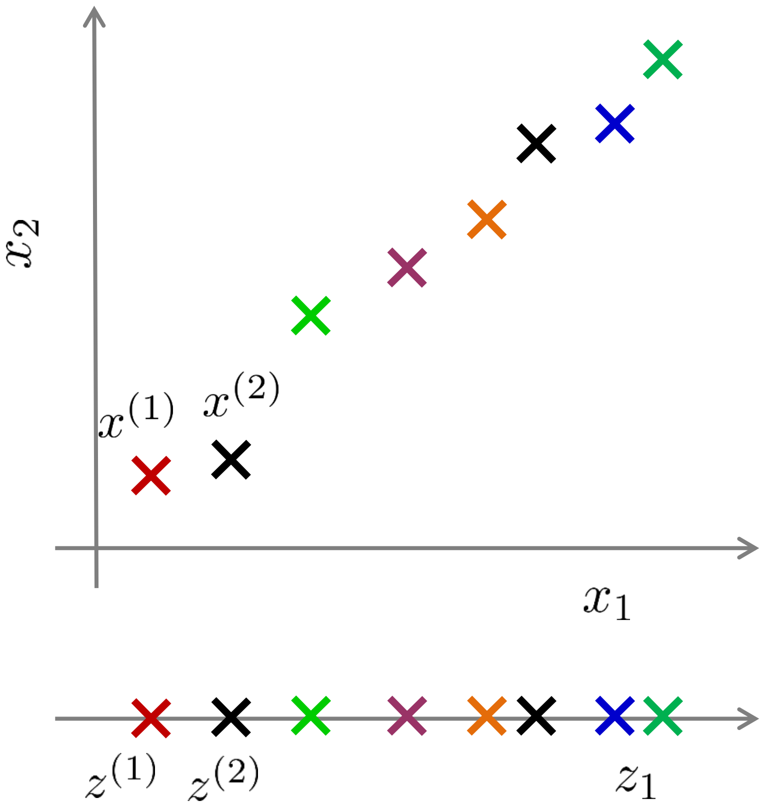
Motivation I:
Data Compression

Data Compression



Reduce data from
2D to 1D

Data Compression



Reduce data from 2D to 1D

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

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

$$\vdots$$

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

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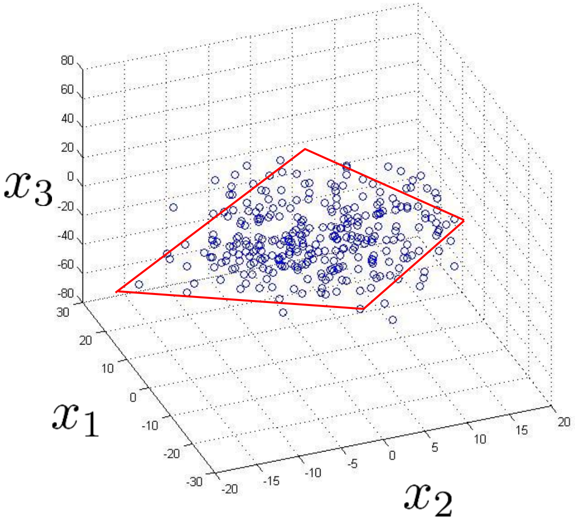
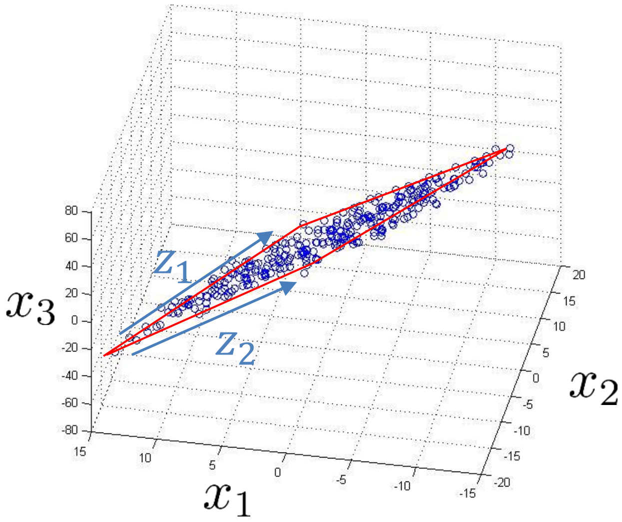
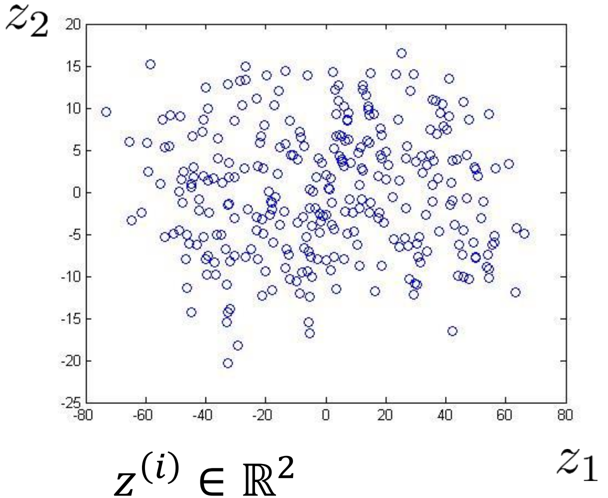
Data Compression

Reduce data from 3D to 2D







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

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

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

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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]

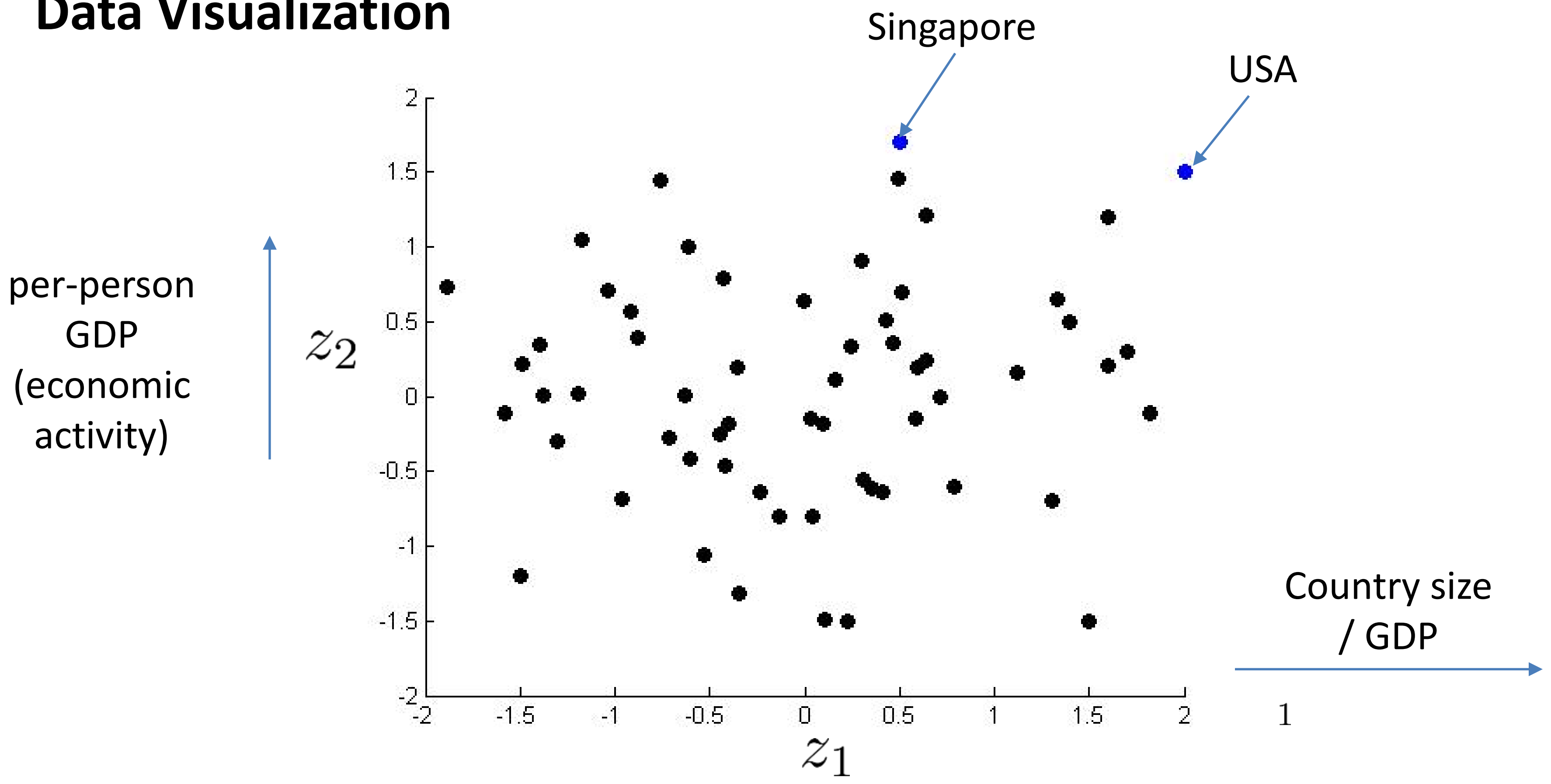
Data Visualization

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

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
…	…	…

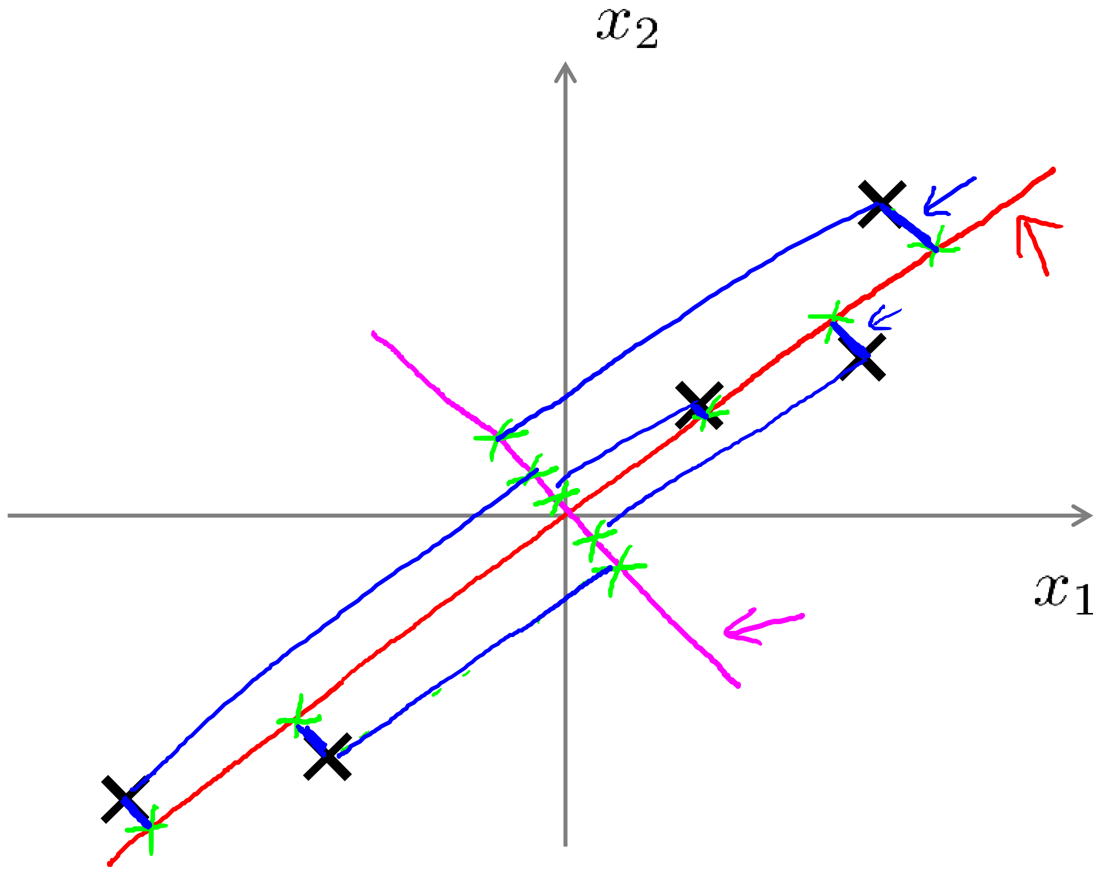
Reduce data from 50D to 2D

Data Visualization

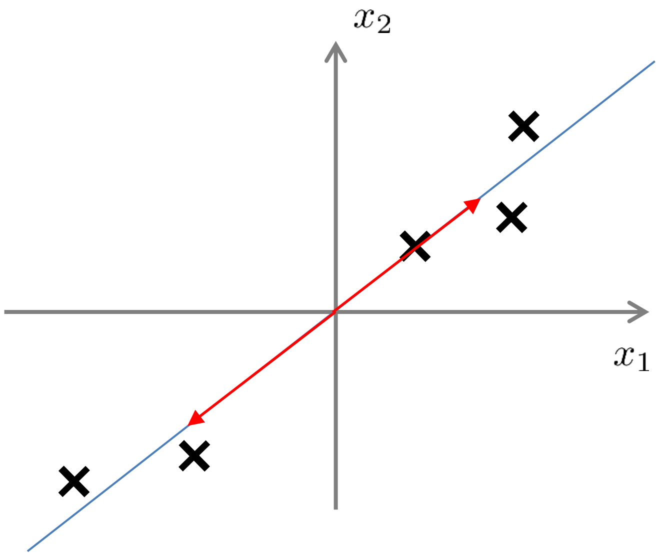


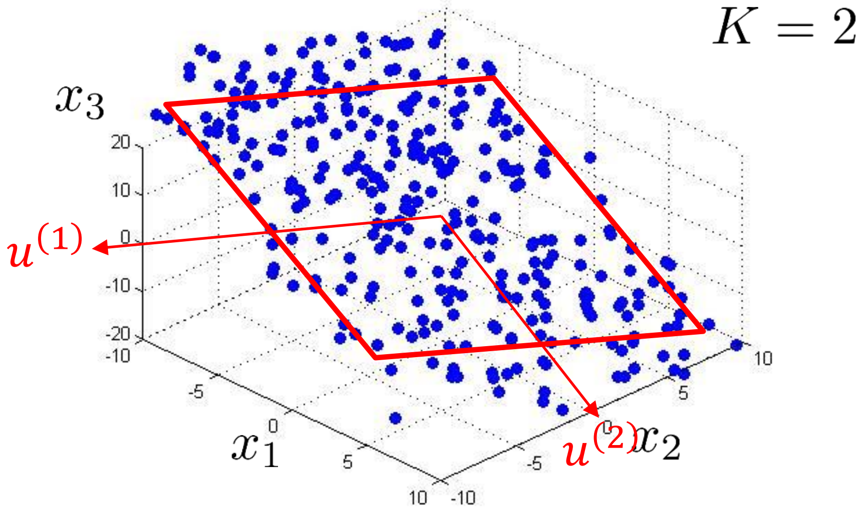
Principal Component Analysis problem formulation

Principal Component Analysis (PCA) problem formulation



Principal Component Analysis (PCA) problem formulation





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.

Principal Component Analysis algorithm

Data preprocessing

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

Preprocessing (feature scaling/mean normalization):

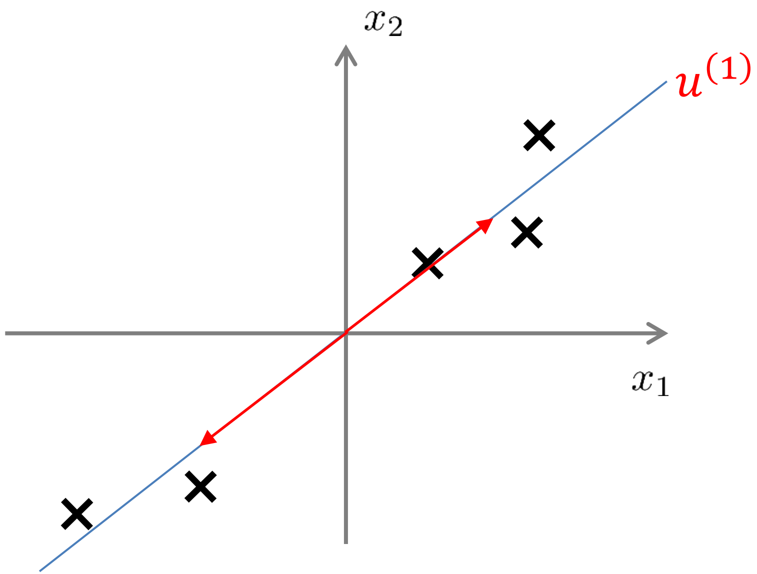
$$\mu_j = \frac{1}{m} \sum_{i=1}^{m} x_j^{(i)}$$

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

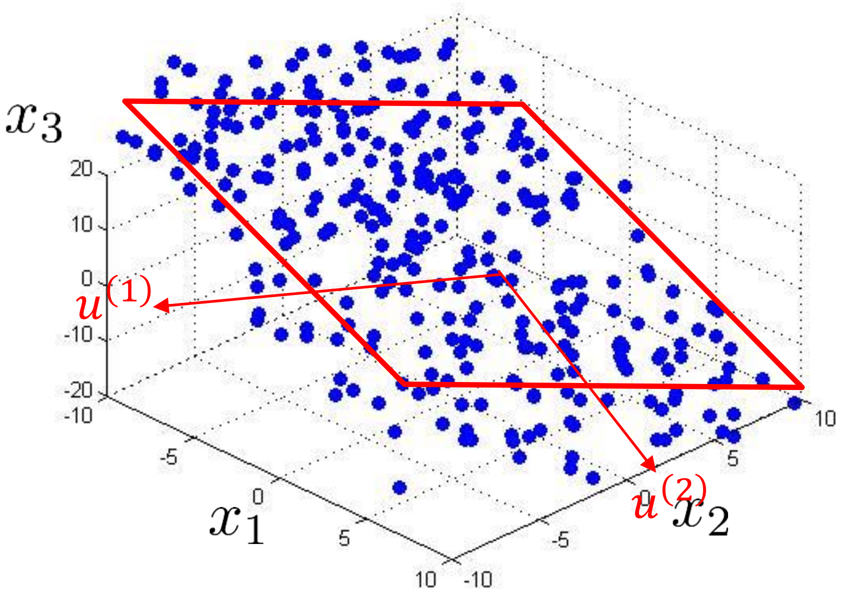
If different features on different scales (e.g., $x_1 =$ size of house, $x_2 =$ number of bedrooms), scale features to have comparable range of values.

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

Principal Component Analysis (PCA) algorithm



Reduce data from 2D to 1D



Reduce data from 3D to 2D

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Principal Component Analysis (PCA) algorithm

Reduce data from n-dimensions to k-dimensions

Compute "covariance matrix":

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

→ Singular value decomposition

Compute "eigenvectors" of matrix Σ:

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

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

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

Principal Component Analysis (PCA) algorithm

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

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

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

Principal Component Analysis (PCA) algorithm summary

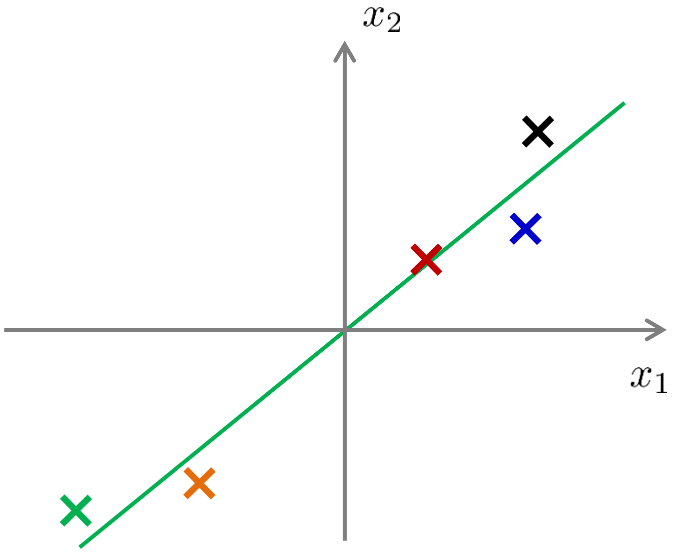
After mean normalization (ensure every feature has zero mean) and optionally feature scaling:

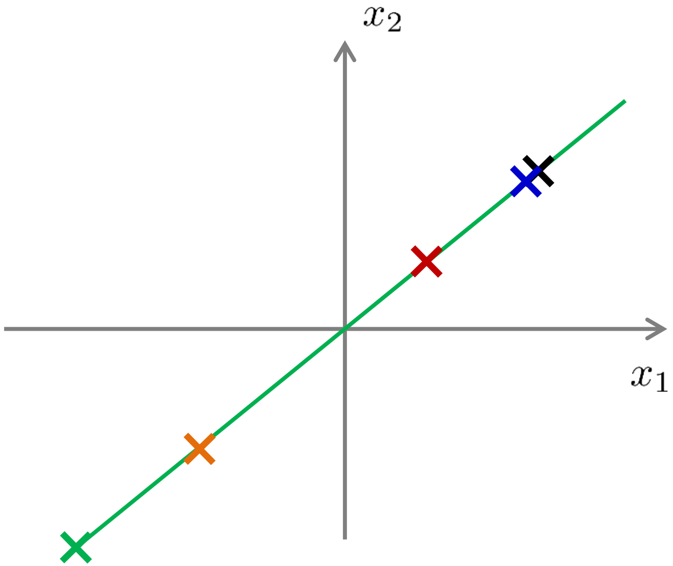
Sigma = $\frac{1}{m}\sum_{i=1}^{m}(x^{(i)})(x^{(i)})^T$

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

Reconstruction from compressed representation

Reconstruction from compressed representation





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

Choosing the number of principal components

Choosing k (number of principal components)

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

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

Typically, choose k to be smallest value so that

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

"99% of variance is retained"

Choosing k (number of principal components)

Algorithm:

Try PCA with $k = 1$

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

Check if

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

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

Choosing k (number of principal components)

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

Pick smallest value of k for which

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

(99% of variance retained)

Advice for applying PCA

Supervised learning speedup

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

Extract inputs:

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

$$\downarrow PCA$$

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

New training set:

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

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.

Application of PCA

- Compression
  - Reduce memory/disk needed to store data
  - Speed up learning algorithm

- Visualization

Bad use of PCA: To prevent overfitting

Use $z^{(i)}$ instead of $x^{(i)}$ to reduce the number of features to $k < n$.

Thus, fewer features, less likely to overfit.

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

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