

~ Principal Component Analysis (PCA) Algorithm ~

Before applying PCA, there is a **data pre-processing** step which we should always do.

Given a training set of m unlabeled examples:

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

It's important to always perform Preprocessing - **feature scaling** / **mean normalization**.

- **Mean Normalization:**

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

- Replace each $x_j^{(i)}$ with $x_j - \mu_j$. In other words, determine the mean of each feature set, and then for each feature subtract the mean from the value, so we re-scale the mean to be 0.

- **Feature Scaling:**

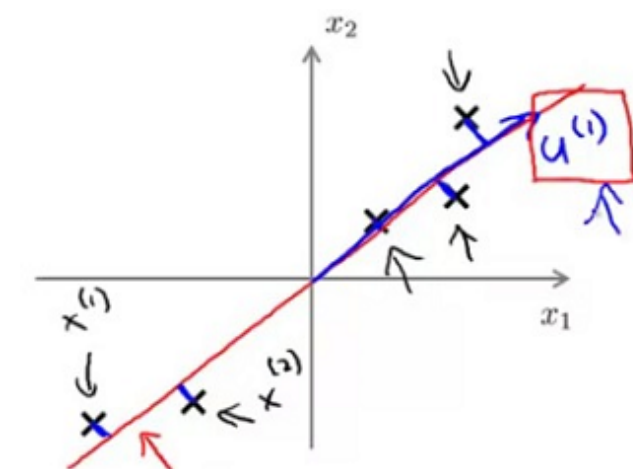
- If different features on different scales (e.g., x_1 = size of house, x_2 = number of bedrooms), scale features to have comparable range of values.

- e.g. $x_j^{(i)}$ is set to $(x_j - \mu_j) / s_j$
- Where s_j is some measure of the range, so could be:
 - Biggest / smallest
 - Standard deviation σ (more commonly)

Having done this sort of data pre-processing, here's what the PCA algorithm does:

We previously saw PCA does is, it tries to find a lower dimensional sub-space onto which to project the data, so as to **minimize sum of the squared projection errors**, and so what we wanted to do specifically is find a vector $u^{(1)}$, which specifies that direction or in the 2D case we want to find two vectors, $u^{(1)}$ and $u^{(2)}$, to define the surface onto which to project the data.

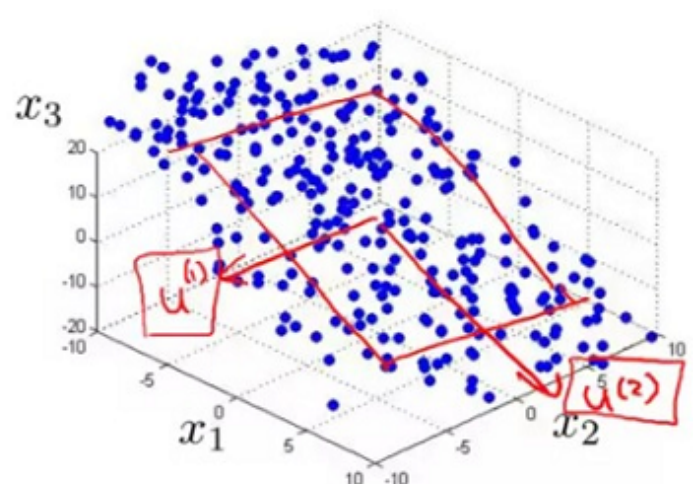
- **Need to compute the z vectors:** z vectors are the new, lower dimensionality feature vectors
- A mathematical derivation for the u vectors is very complicated
 - But once we've done it, the procedure to find each u vector is not that hard.



Reduce data from 2D to 1D

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

A 1D plot showing the reduced data points $z^{(1)}$ and $z^{(2)}$ along a horizontal axis. A vector z_1 is shown pointing along this axis.



Reduce data from 3D to 2D

$$x^{(i)} \in \mathbb{R}^3 \rightarrow z^{(i)} \in \mathbb{R}^2$$
$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

PCA Algorithm description:

Reduce data from n -dimensions to k -dimensions

- Compute "covariance matrix":

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

This is commonly denoted as Σ (greek upper case sigma) - NOT summation symbol

- This is an $[n \times n]$ matrix
 - Remember that $x^{(1)}$ is a $[n \times 1]$ matrix

Compute "eigenvectors" of matrix Σ :

- On octave, the way we do that is to use the command: **[U,S,V] = svd(sigma)**
 - SVD stands for **singular value decomposition**.
 - More numerically stable than eig
 - **eig** = also gives a eigenvector

Compute "covariance matrix":

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

Compute "eigenvectors" of matrix Σ :

$$\rightarrow [U, S, V] = \text{svd}(\text{Sigma}); \quad \rightarrow \text{Singular value decomposition eig}(\text{Sigma})$$

$n \times n$ matrix.

And what the SVD outputs three matrices, U , S , and V . The thing we really need out of the SVD is the u matrix.

- U matrix is also an $[n \times n]$ matrix ($U \in \mathbb{R}^{n \times n}$)
- Turns out the columns of U are the u vectors we want
 - So to reduce a system from n -dimensions to k -dimensions
 - Just take the first k -vectors from U (first k columns)

From **[U,S,V] = svd(sigma)**, we get:

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

$\underbrace{\hspace{10em}}_k$
 $x \in \mathbb{R}^n \rightarrow z \in \mathbb{R}^k$

Next we need to find some way to change x (which is n dimensional) to z (which is k dimensional)
 $x \in \mathbb{R}^n \rightarrow z \in \mathbb{R}^k$ (reduce the dimensionality).

- Take first k columns of the U matrix and stack in columns
 - $n \times k$ matrix - call this U_{reduce}

We calculate z as follows:

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

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

$z \in \mathbb{R}^k$ $k \times 1$

- So $U_{\text{reduce}}^T * x^{(i)}$ which is $[k \times n] * [n \times 1]$
- Generates a matrix which is $[k \times 1] = z^{(i)}$

Principal Component Analysis (PCA) algorithm summary

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

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

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

- Calculate sigma (covariance matrix Σ)
 - In MATLAB or octave we can implement this as follows:
 - **sigma = (1 / m) * (X' * X);**
- Next we can apply SVD (Singular Value Decomposition) routine to calculate the eigenvectors U, S, V
 - Take k vectors from U :
 - **Ureduce = U(:, 1:k);**
- Finally calculate z :
 - **z = Ureduce' * x;**

Video Question: In PCA, we obtain $z \in \mathbb{R}^k$ from $x \in \mathbb{R}^n$ as follows:

$$z = \begin{bmatrix} | & | & \dots & | \\ u^{(1)} & u^{(2)} & \dots & u^{(k)} \\ | & | & \dots & | \end{bmatrix}^T x = \begin{bmatrix} \text{---} (u^{(1)})^T \text{---} \\ \text{---} (u^{(2)})^T \text{---} \\ \vdots \\ \text{---} (u^{(k)})^T \text{---} \end{bmatrix} x$$

Which of the following is a correct expression for z_j ?

- $z_j = (u^{(k)})^T x$
- $z_j = (u^{(j)})^T x_j$
- $z_j = (u^{(j)})^T x_k$

$$z_j = (u^{(j)})^T x$$