# 13: Clustering





## Unsupervised learning - introduction

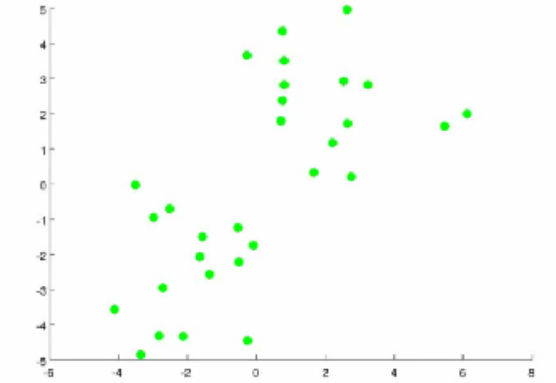
- Talk about **clustering**
  - **Learning from unlabeled data**
- Unsupervised learning
  - Useful to contras with supervised learning
- Compare and contrast
  - Supervised learning
    - Given a set of labels, fit a hypothesis to it
  - Unsupervised learning
    - Try and determining structure in the data
    - Clustering algorithm groups data together based on data features
- What is clustering good for
  - **Market segmentation** - group customers into different market segments
  - **Social network analysis** - Facebook "smartlists"
  - **Organizing computer clusters** and data centers for network layout and location
  - **Astronomical data analysis** - Understanding galaxy formation

## K-means algorithm

- Want an algorithm to automatically group the data into coherent clusters
- K-means is **by far** the most widely used clustering algorithm

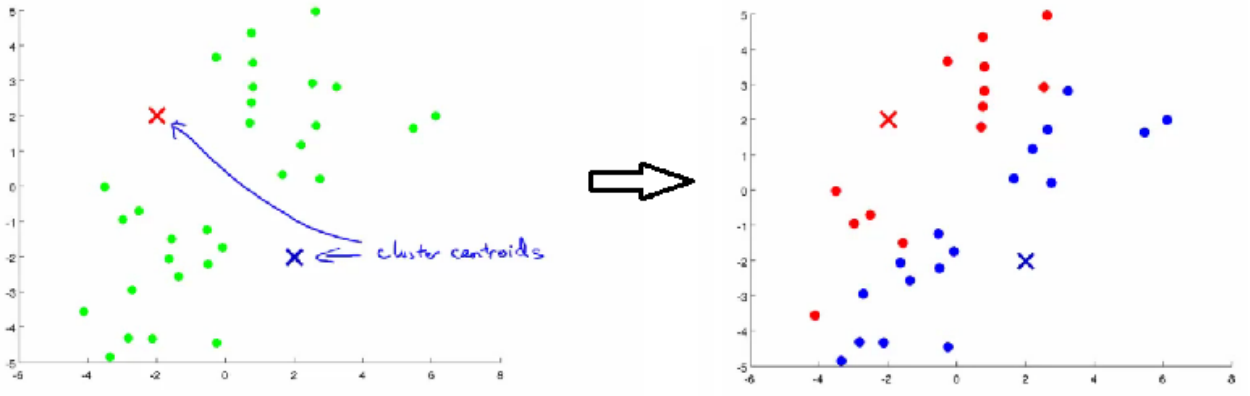
### Overview

- Take unlabeled data and group into two clusters

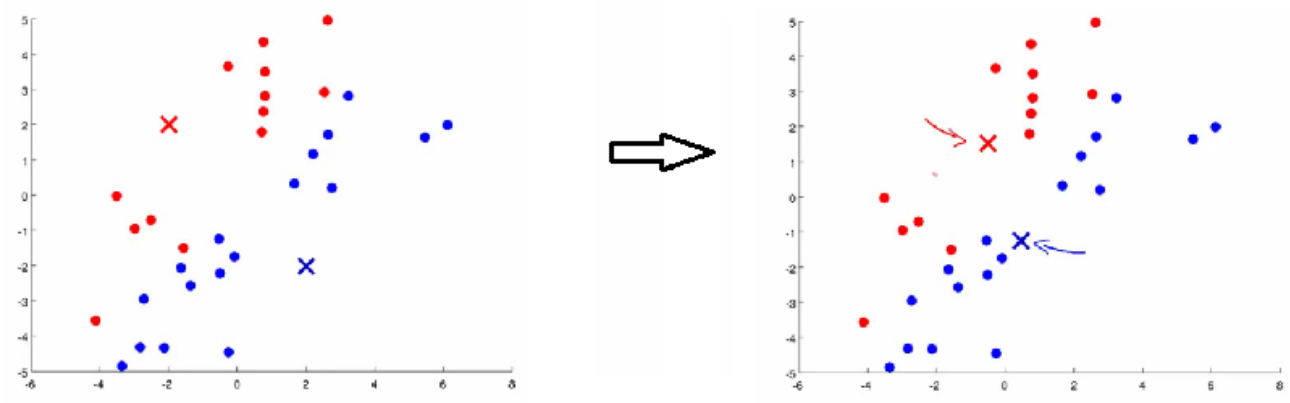


- Algorithm overview
  - 1) Randomly allocate two points as the **cluster centroids**
    - Have as many cluster centroids as clusters you want to do (*K* cluster centroids, in fact)
    - In our example we just have two clusters
  - 2) Cluster assignment step
    - Go through each example and depending on if it's closer to the red or blue centroid assign each point to one of the two clusters

- To demonstrate this, we've gone through the data and "colour" each point red or blue




- 3) Move centroid step
  - Take each centroid and move to the average of the correspondingly assigned data-points



  - Repeat 2) and 3) until convergence
- More formal definition
  - **Input:**
    - K (number of clusters in the data)
    - Training set $\{x^1, x^2, x^3 \ldots, x^n)$
  - **Algorithm:**
    - Randomly initialize K cluster centroids as $\{\mu_1, \mu_2, \mu_3 \ldots \mu_K\}$

```
Repeat {
        for i = 1 to m
            c(i) := index (from 1 to K) of cluster centroid
                    closest to x(i)
        for k = 1 to K
            μk := average (mean) of points assigned to cluster k }
```

      - Loop 1
        - This inner loop repeatedly sets the $c^{(i)}$ variable to be the index of the closes variable of cluster centroid closes to $x^i$
        - i.e. take $i^{th}$ example, measure squared distance to each cluster centroid, assign $c^{(i)}$to the cluster closest

$$\min_k \|x^{(i)} - \mu_k\|^2 \rightarrow c^{(i)}$$

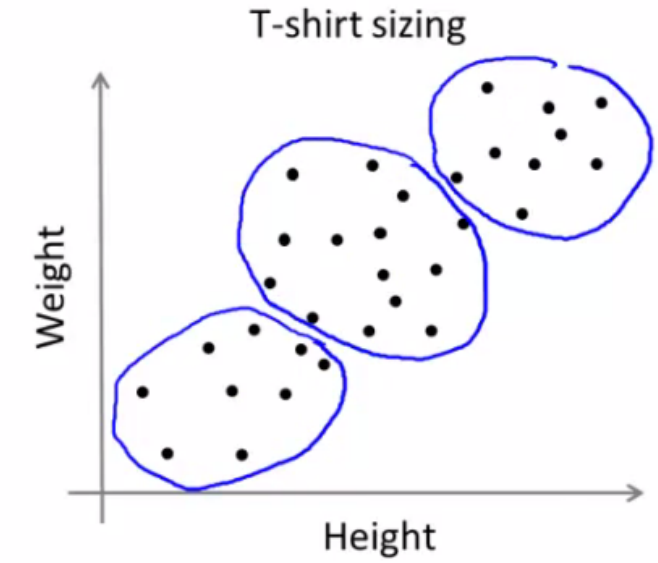
      - Loop 2
        - Loops over each centroid calculate the average mean based on all the points associated with each centroid from $c^{(i)}$

        - What if there's a centroid with no data
            - Remove that centroid, so end up with K-1 classes
            - Or, randomly reinitialize it
                - Not sure when though...

**K-means for non-separated clusters**

- So far looking at K-means where we have well defined clusters
- But often K-means is applied to datasets where there aren't well defined clusters
    - e.g. T-shirt sizing


- Not obvious discrete groups
- Say you want to have three sizes (S,M,L) how big do you make these?
    - One way would be to run K-means on this data
    - May do the following




    - So creates three clusters, even though they aren't really there
    - Look at first population of people
        - Try and design a small T-shirt which fits the 1st population
        - And so on for the other two
    - This is an example of market segmentation
        - Build products which suit the needs of your subpopulations

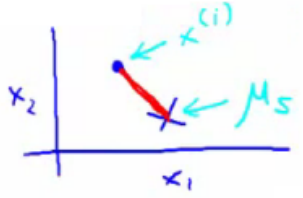
# K means optimization objective

- Supervised learning algorithms have an optimization objective (cost function)
    - K-means does too
- K-means has an optimization objective like the supervised learning functions we've seen

    - Why is this good?
    - Knowing this is useful because it helps for debugging
    - Helps find better clusters
- While K-means is running we keep track of two sets of variables
    - $c^i$ is the index of clusters {1,2, ..., K} to which $x^i$ is currently assigned
        - i.e. there are *m* $c^i$ values, as each example has a $c^i$ value, and that value is one the the clusters (i.e. can only be one of K different values)
    - $\mu_k$, is the cluster associated with centroid *k*
        - Locations of cluster centroid k
        - So there are K
        - So these the centroids which exist in the training data space
    - $\mu_c^i$, is the cluster centroid of the cluster to which example $x^i$ has been assigned to
        - This is more for convenience than anything else
            - You could look up that example i is indexed to cluster j (using the c vector), where j is between 1 and K
            - Then look up the value associated with cluster j in the μ vector (i.e. what are the features associated with $\mu_j$)
            - But instead, for easy description, we have this variable which gets exactly the same value
        - Lets say $x^i$ as been assigned to cluster 5
            - Means that
                - $c^i = 5$
                - $\mu_c^i, = \mu_5$
- Using this notation we can write the optimization objective;

$$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K) = \frac{1}{m} \sum_{i=1}^{m} ||x^{(i)} - \mu_{c^{(i)}}||^2$$

    - i.e. squared distances between training example $x^i$ and the cluster centroid to which $x^i$ has been assigned to
        - This is just what we've been doing, as the visual description below shows;




        - The red line here shows the distances between the example $x^i$ and the cluster to which that example has been assigned
            - Means that when the example is very close to the cluster, this value is small
            - When the cluster is very far away from the example, the value is large
    - This is sometimes called the **distortion** (or **distortion cost function**)
    - So we are finding the values which minimizes this function;

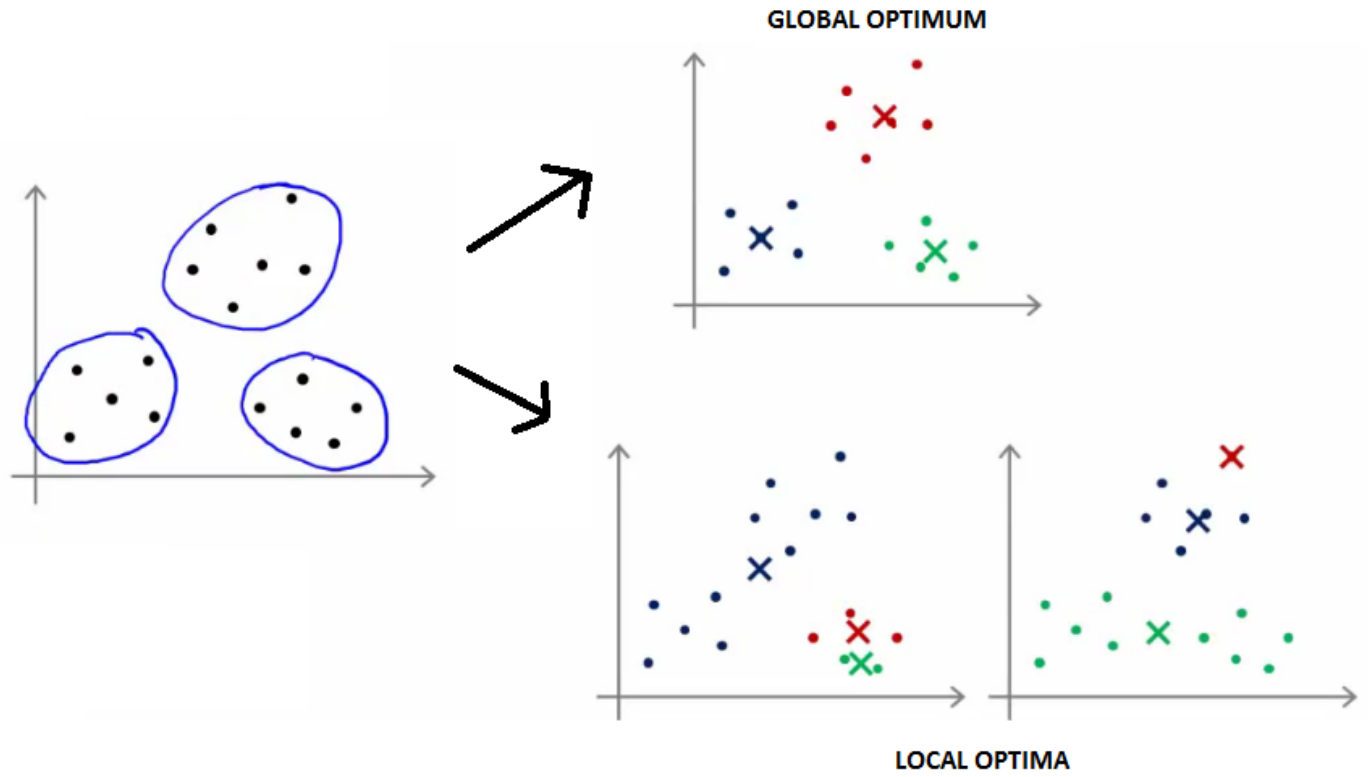
$$\min_{\substack{c^{(1)},\ldots,c^{(m)},\\ \mu_1,\ldots,\mu_K}} J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$$

- If we consider the k-means algorithm
    - The **cluster assigned step** is minimizing J(...) with respect to $c^1$, $c^2$ ... $c^i$
        - i.e. find the centroid closest to each example
        - Doesn't change the centroids themselves
    - The **move centroid step**
        - We can show this step is choosing the values of μ which minimizes J(...) with respect to μ
    - So, we're partitioning the algorithm into two parts
        - First part minimizes the c variables
        - Second part minimizes the J variables
- We can use this knowledge to help debug our K-means algorithm

### Random initialization

- How we initialize K-means
    - And how avoid local optimum

- Consider clustering algorithm
  - Never spoke about how we initialize the centroids
    - A few ways - one method is most recommended
- Have number of centroids set to less than number of examples (K < m) (if K > m we have a problem)0
  - Randomly pick K training examples
  - Set $\mu_1$ up to $\mu_K$ to these example's values
- K means can converge to different solutions depending on the initialization setup
  - Risk of local optimum




  - The local optimum are valid convergence, but local optimum not global ones
- If this is a concern
  - We can do multiple random initializations
    - See if we get the same result - many same results are likely to indicate a global optimum
- Algorithmically we can do this as follows;

For i = 1 to 100 {
Randomly initialize K-means.
Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$
Compute cost function (distortion)
$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$ }

  - A typical number of times to initialize K-means is 50-1000
  - Randomly initialize K-means
    - For each 100 random initialization run K-means
    - Then compute the distortion on the set of cluster assignments and centroids at convergent
    - End with 100 ways of cluster the data
    - Pick the clustering which gave the lowest distortion
- If you're running K means with 2-10 clusters can help find better global optimum
  - If K is larger than 10, then multiple random initializations are less likely to be necessary
  - First solution is probably good enough (better granularity of clustering)

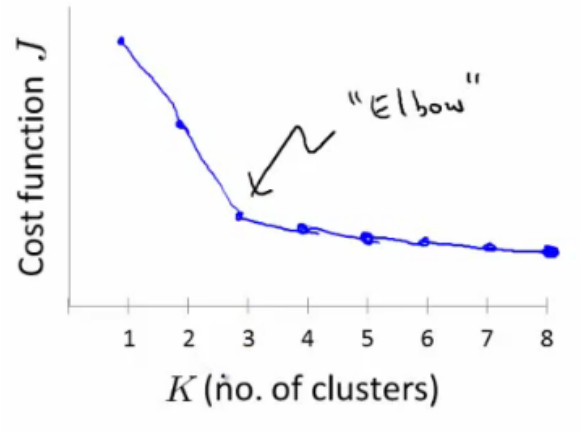
# How do we choose the number of clusters?

- Choosing K?
  - Not a great way to do this automatically
  - Normally use visualizations to do it manually
- What are the intuitions regarding the data?
- Why is this hard

- Sometimes very ambiguous
  - e.g. two clusters or four clusters
  - Not necessarily a correct answer
- This is why doing it automatic this is hard

### Elbow method

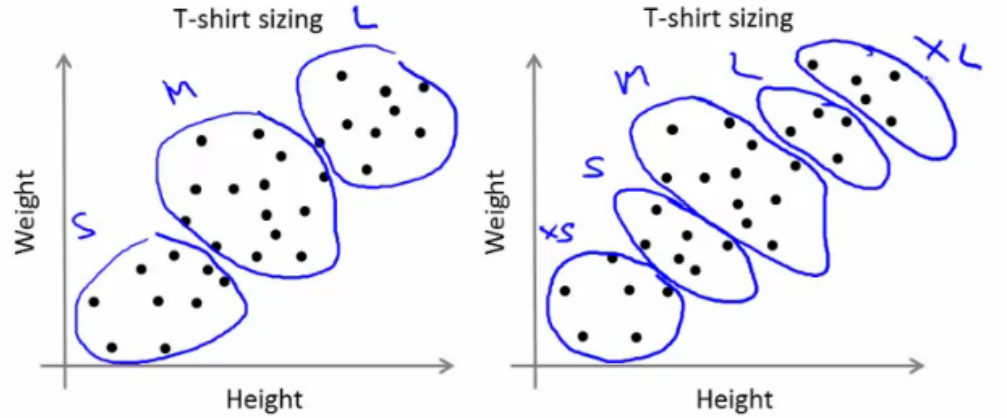
- Vary K and compute cost function at a range of K values
- As K increases J(...) minimum value should decrease (i.e. you decrease the granularity so centroids can better optimize)
  - Plot this (K vs J())
- Look for the "elbow" on the graph




- Chose the "elbow" number of clusters
- If you get a nice plot this is a reasonable way of choosing K
- Risks
  - Normally you don't get a a nice line -> no clear elbow on curve
  - Not really that helpful

### Another method for choosing K

- Using K-means for market segmentation
- Running K-means for a later/downstream purpose
  - See how well different number of clusters serve you later needs
- e.g.
  - T-shirt size example
    - If you have three sizes (S,M,L)
    - Or five sizes (XS, S, M, L, XL)
    - Run K means where K = 3 and K = 5
  - How does this look




  - This gives a way to chose the number of clusters
    - Could consider the cost of making extra sizes vs. how well distributed the products are
    - How important are those sizes though? (e.g. more sizes might make the customers happier)
    - So applied problem may help guide the number of clusters

# 14: Dimensionality Reduction (PCA)

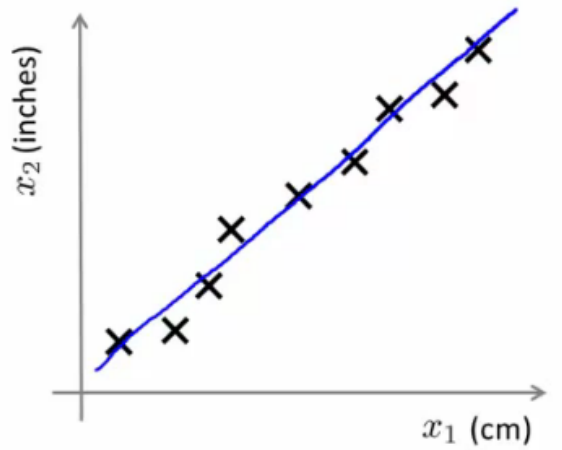


## Motivation 1: Data compression

- Start talking about a second type of unsupervised learning problem - **dimensionality reduction**
  - Why should we look at dimensionality reduction?

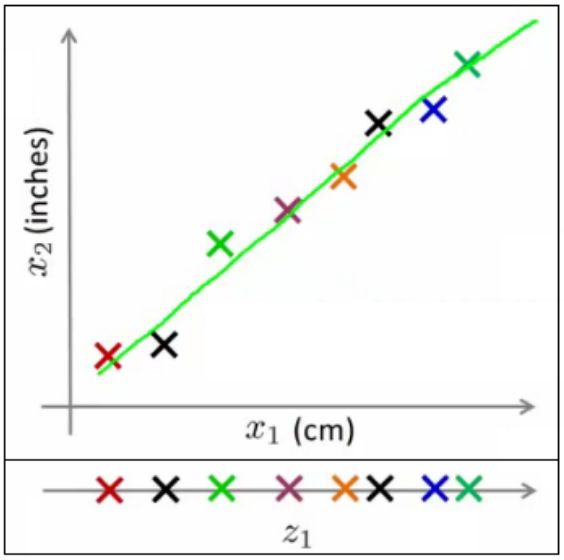
**Compression**

- Speeds up algorithms
- Reduces space used by data for them
- What is dimensionality reduction?
  - So you've collected many features - maybe more than you need
    - Can you "simply" your data set in a rational and useful way?
  - Example
    - Redundant data set - different units for same attribute
    - Reduce data to 1D (2D->1D)

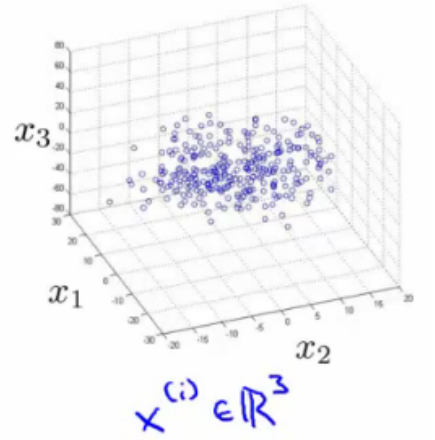



    - Example above isn't a perfect straight line because of round-off error
  - Data redundancy can happen when different teams are working independently
    - Often generates redundant data (especially if you don't control data collection)
  - Another example
    - Helicopter flying - do a survey of pilots (x1 = skill, x2 = pilot enjoyment)
      - These features may be highly correlated
      - This correlation can be combined into a single attribute called aptitude (for example)

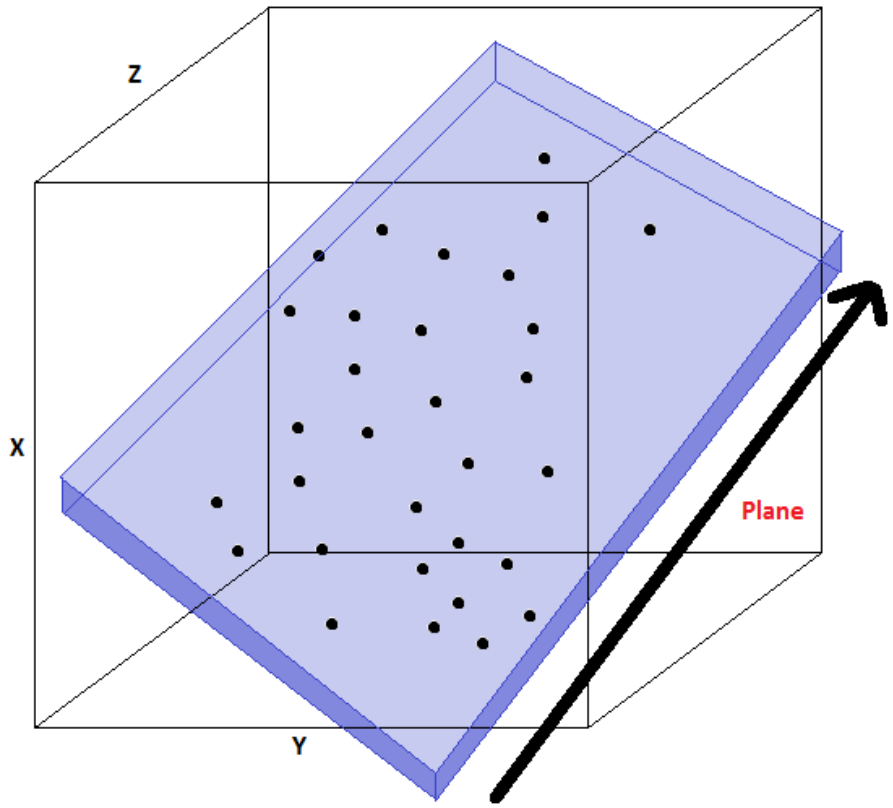
- What does dimensionality reduction mean?
  - In our example we plot a line
  - Take exact example and record position on that line



    - So before $x^1$ was a 2D feature vector (X and Y dimensions)
    - Now we can represent $x^1$ as a 1D number (Z dimension)
- So we approximate original examples
    - Allows us to half the amount of storage
    - Gives lossy compression, but an acceptable loss (probably)
        - The loss above comes from the rounding error in the measurement, however
- Another example 3D -> 2D
    - So here's our data

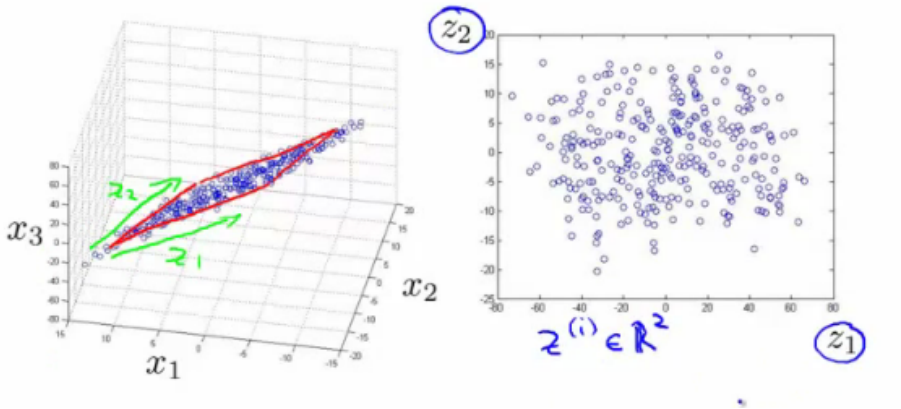



    - Maybe all the data lies in one plane
        - This is sort of hard to explain in 2D graphics, but that plane may be aligned with one of the axis
            - Or or may not...
            - Either way, the plane is a small, a constant 3D space
        - In the diagram below, imagine all our data points are sitting "inside" the blue tray (has a dark blue exterior face and a light blue inside)




        - Because they're all in this relative shallow area, we can basically ignore one of the dimension, so we draw two new lines (z1 and z2) along the x and y planes of the box, and plot the locations in that box
        - i.e. we loose the data in the z-dimension of our "shallow box" (NB "z-dimensions" here refers to the dimension relative to the box (i.e it's depth) and NOT the z dimension of the axis we've got drawn above) but because the box is shallow it's OK to lose this. Probably....

- Plot values along those projections




  - So we've now reduced our 3D vector to a 2D vector
- In reality we'd normally try and do 1000D -> 100D

# Motivation 2: Visualization

- It's hard to visualize highly dimensional data
  - Dimensionality reduction can improve how we display information in a tractable manner for human consumption
  - Why do we care?
    - Often helps to develop algorithms if we can understand our data better
    - Dimensionality reduction helps us do this, see data in a helpful
    - Good for explaining something to someone if you can "show" it in the data
- Example;
  - Collect a large data set about many facts of a country around the world

| Country | GDP (trillions of US$) | Per capita GDP (thousands of intl. $) | Human Develop-ment Index | Life expectancy | Poverty Index (Gini as percentage) | Mean household income (thousands of US$) | ... |
|---|---|---|---|---|---|---|---|
| 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 | ... |
| ... | ... | ... | ... | ... | ... | ... | |

    - So
      - $x_1$ = GDP
      - ...
      - $x_6$ = mean household
    - Say we have 50 features per country
    - How can we understand this data better?
      - Very hard to plot 50 dimensional data
  - Using dimensionality reduction, instead of each country being represented by a 50-dimensional feature vector

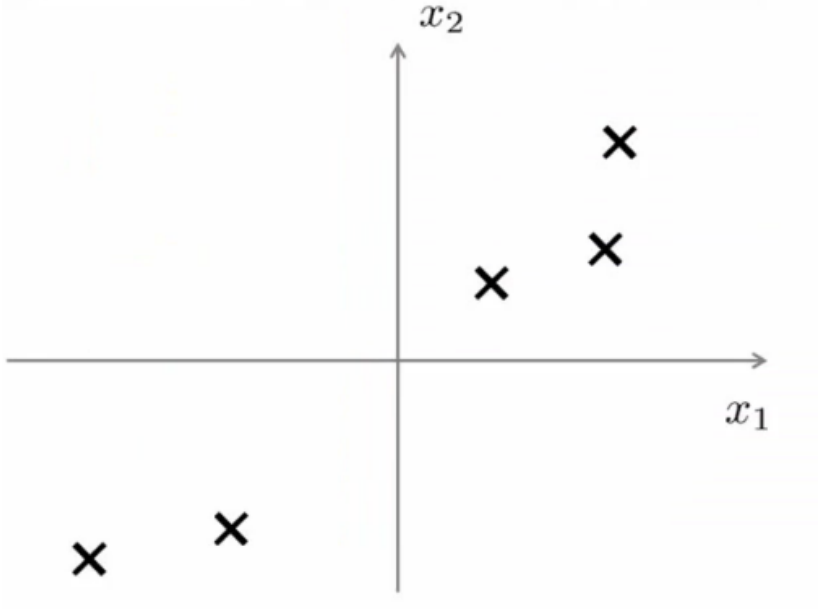
- Come up with a different feature representation (z values) which summarize these features

| 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 |
| ... | ... | ... |

  - This gives us a 2-dimensional vector
    - Reduce 50D -> 2D
    - Plot as a 2D plot
  - Typically you don't generally ascribe meaning to the new features (so we have to determine what these summary values mean)
    - e.g. may find horizontal axis corresponds to overall country size/economic activity
    - and y axis may be the per-person well being/economic activity
  - So despite having 50 features, there may be two "dimensions" of information, with features associated with each of those dimensions
    - It's up to you to asses what of the features can be grouped to form summary features, and how best to do that (feature scaling is probably important)
  - Helps show the two main dimensions of variation in a way that's easy to understand

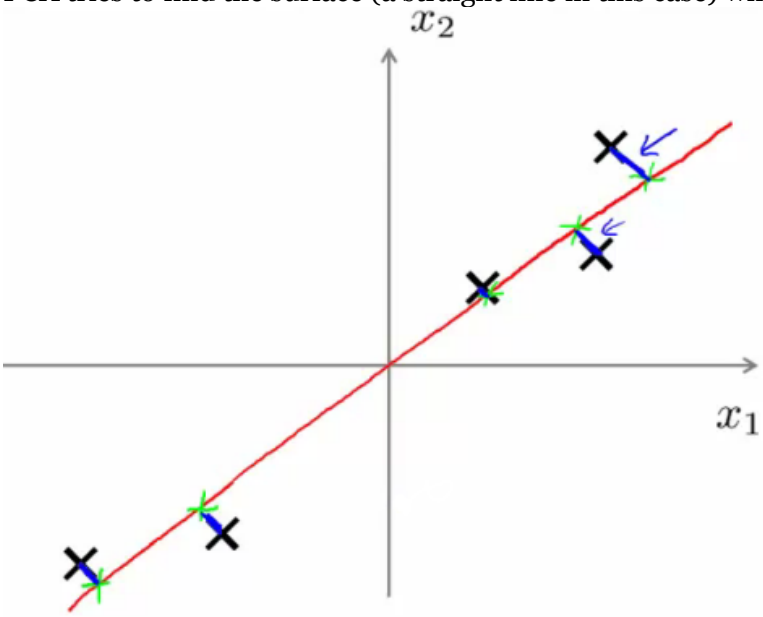
# Principle Component Analysis (PCA): Problem Formulation

- For the problem of dimensionality reduction the most commonly used algorithm is **PCA**
  - Here, we'll start talking about how we formulate precisely what we want PCA to do
- So
  - Say we have a 2D data set which we wish to reduce to 1D

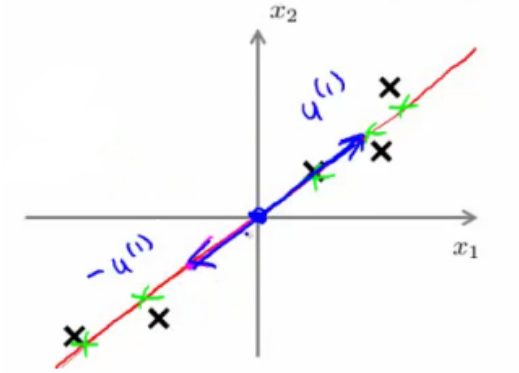



  - In other words, find a single line onto which to project this data
    - How do we determine this line?

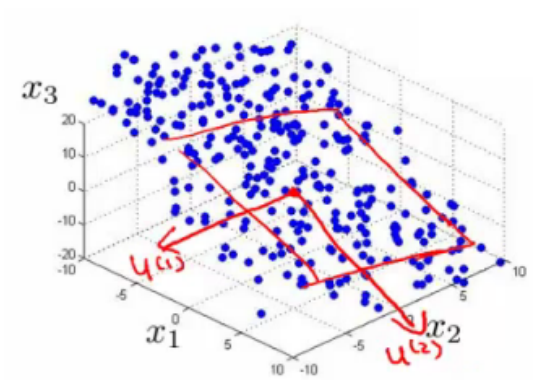
        - The distance between each point and the projected version should be small (blue lines below are short)
        - PCA tries to find a lower dimensional surface so the sum of squares onto that surface is minimized
        - The blue lines are sometimes called the **projection error**
            - PCA tries to find the surface (a straight line in this case) which has the minimum projection error




        - As an aside, you should normally do **mean normalization** and **feature scaling** on your data before PCA
- A more formal description is
    - For 2D-1D, we must find a vector $u^{(1)}$, which is of some dimensionality
    - Onto which you can project the data so as to minimize the projection error



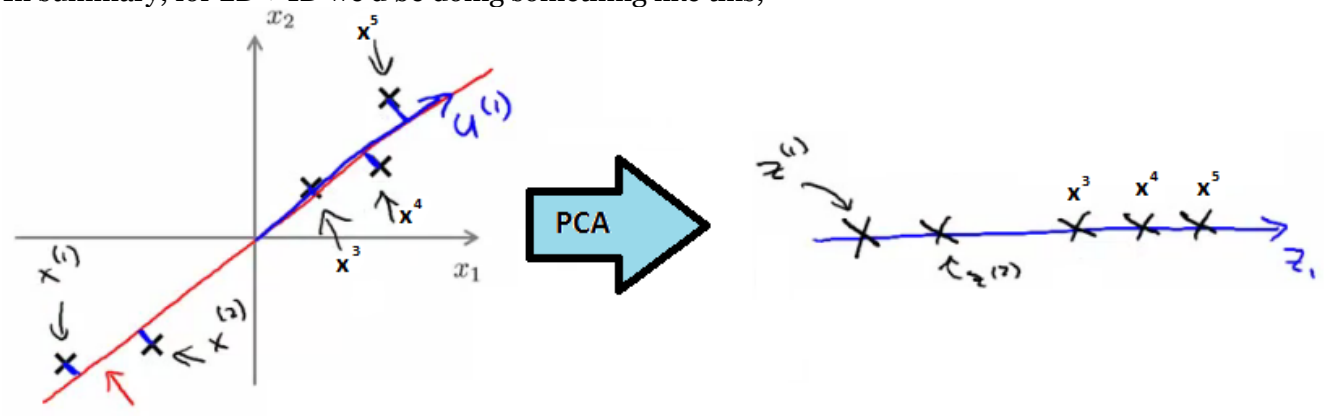

    - $u^{(1)}$ can be positive or negative ($-u^{(1)}$) which makes no difference
        - Each of the vectors define the same red line
- In the more general case
    - To reduce from nD to kD we
        - Find *k* vectors ($u^{(1)}$, $u^{(2)}$, ... $u^{(k)}$) onto which to project the data to minimize the projection error
        - So lots of vectors onto which we project the data
        - Find a set of vectors which we project the data onto the linear subspace spanned by that set of vectors
            - We can define a point in a plane with k vectors
    - e.g. 3D->2D
        - Find pair of vectors which define a 2D plane (surface) onto which you're going to project your data
        - Much like the "shallow box" example in compression, we're trying to create the shallowest box possible (by defining two of it's three dimensions, so the box' depth is minimized)




- How does PCA relate to linear regression?
  - PCA is **not** linear regression
    - Despite cosmetic similarities, very different
  - For linear regression, fitting a straight line to minimize the **straight line** between a point and a squared line
    - NB - **VERTICAL distance** between point
  - For PCA minimizing the magnitude of the shortest **orthogonal distance**
    - Gives very different effects
  - More generally
    - With linear regression we're trying to predict "y"
    - With PCA there is no "y" - instead we have a list of features and all features are treated equally
      - If we have 3D dimensional data 3D->2D
        - Have 3 features treated symmetrically

# PCA Algorithm

- Before applying PCA must do data preprocessing
  - Given a set of m unlabeled examples we must do
    - **Mean normalization**
      - 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 (depending on data)**
      - If features have very different scales then scale so they all have a 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 (more commonly)
- With preprocessing done, PCA finds the lower dimensional sub-space which minimizes the sum of the square
  - In summary, for 2D->1D we'd be doing something like this;




  - Need to compute two things;
    - Compute the **u vectors**
      - The new planes
    - 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 you've done it, the procedure to find each u vector is not that hard

**Algorithm description**

- Reducing data from *n*-dimensional to k-dimensional
  - Compute the 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
    - Σ = sigma
      - This is an [n x n] matrix
        - Remember than $x^i$ is a [n x 1] matrix
    - In MATLAB or octave we can implement this as follows;

```
sigma = (1/m) * ( X' * X )
```

  - Compute eigenvectors of matrix Σ
    - `[U,S,V] = svd(sigma)`
      - svd = singular value decomposition
        - More numerically stable than `eig`
      - `eig` = also gives eigenvector
  - U,S and V are matrices
    - U matrix is also an [n x n] matrix
    - 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)

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

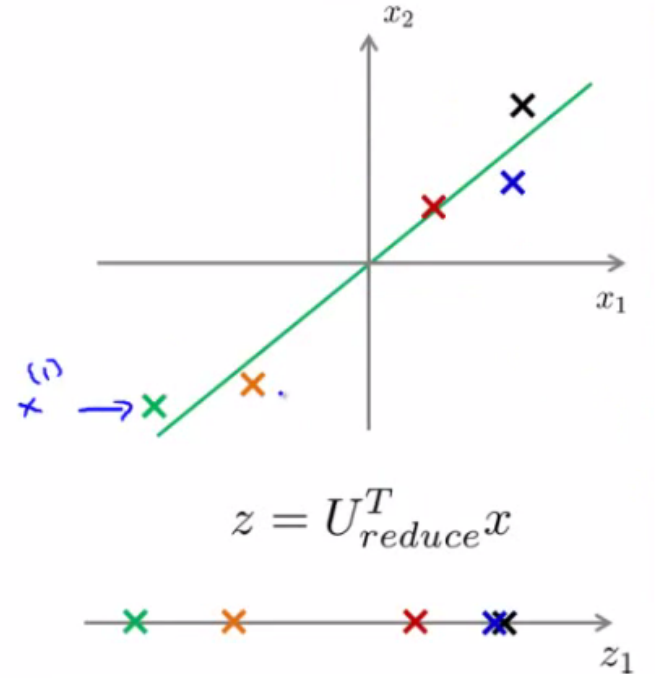
- Next we need to find some way to change x (which is n dimensional) to z (which is k dimensional)
  - (reduce the dimensionality)
  - Take first k columns of the u matrix and stack in columns
    - n x k matrix - call this $U_{reduce}$
  - We calculate z as follows
    - $z = (U_{reduce})^T * x$
      - So [k x n] * [n x 1]
      - Generates a matrix which is
        - k * 1
      - If that's not witchcraft I don't know what is!

- Exactly the same as with supervised learning except we're now doing it with unlabeled data
- So in summary
  - Preprocessing
  - Calculate sigma (covariance matrix)
  - Calculate eigenvectors with **svd**
  - Take k vectors from U ($U_{reduce}$= U(:,1:k);)
  - Calculate z ($z = U_{reduce}' * x$;)
- No mathematical derivation
  - Very complicated
  - But it works

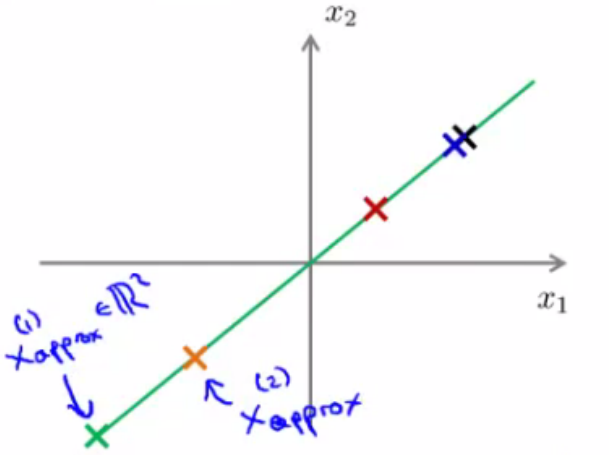
# Reconstruction from Compressed Representation

- Earlier spoke about PCA as a compression algorithm
  - If this is the case, is there a way to **decompress** the data from low dimensionality back to a higher dimensionality format?
- Reconstruction

- Say we have an example as follows




  - We have our examples ($x^1$, $x^2$ etc.)
  - Project onto z-surface
  - Given a point $z^1$, how can we go back to the 2D space?
- Considering
  - z (vector) = $(U_{reduce})^T * x$
- To go in the opposite direction we must do
  - $x_{approx} = U_{reduce} * z$
    - To consider dimensions (and prove this really works)
      - $U_{reduce}$ = [n x k]
      - z [k * 1]
    - So
      - $x_{approx}$ = [n x 1]
- So this creates the following representation



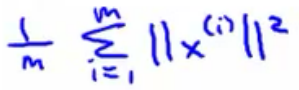

- We lose some of the information (i.e. everything is now perfectly on that line) but it is now projected into 2D space

# Choosing the number of Principle Components

- How do we chose *k* ?
  - k = number of **principle components**
  - Guidelines about how to chose k for PCA
- To chose k think about how PCA works

- PCA tries to minimize averaged squared projection error

- Total variation in data can be defined as the average over data saying how far are the training examples from the origin



- When we're choosing k typical to use something like this

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

  - Ratio between averaged squared projection error with total variation in data
    - Want ratio to be small - means we retain 99% of the variance
  - If it's small (0) then this is because the numerator is small
    - The numerator is small when $x^i = x_{approx}{}^i$
      - i.e. we lose very little information in the dimensionality reduction, so when we decompress we regenerate the same data
- So we chose k in terms of this ratio
- Often can significantly reduce data dimensionality while retaining the variance
- How do you do this

Algorithm:

Try PCA with $k = 1$

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

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

# Advice for Applying PCA

- Can use PCA to speed up algorithm running time
  - Explain how
  - And give general advice

### Speeding up supervised learning algorithms

- Say you have a supervised learning problem
  - Input x and y
    - x is a 10 000 dimensional feature vector
    - e.g. 100 x 100 images = 10 000 pixels
    - Such a huge feature vector will make the algorithm slow
  - With PCA we can reduce the dimensionality and make it tractable
  - How
    - 1) Extract xs
      - So we now have an unlabeled training set
    - 2) Apply PCA to x vectors
      - So we now have a reduced dimensional feature vector z
    - 3) This gives you a new training set
      - Each vector can be re-associated with the label

        - 4) Take the reduced dimensionality data set and feed to a learning algorithm
            - Use y as labels and z as feature vector
        - 5) If you have a new example map from higher dimensionality vector to lower dimensionality vector, then feed into learning algorithm
- PCA maps one vector to a lower dimensionality vector
    - x -> z
    - Defined by PCA **only** on the training set
    - The mapping computes a set of parameters
        - Feature scaling values
        - $U_{reduce}$
            - Parameter learned by PCA
            - Should be obtained only by determining PCA on your training set
    - So we use those learned parameters for our
        - Cross validation data
        - Test set
- Typically you can reduce data dimensionality by 5-10x without a major hit to algorithm

# Applications of PCA

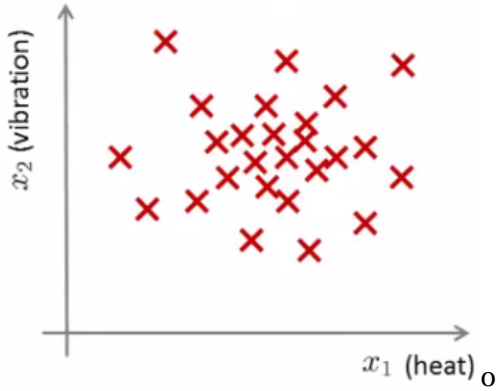
- **Compression**
    - Why
        - Reduce memory/disk needed to store data
        - Speed up learning algorithm
    - How do we chose k?
        - % of variance retained
- **Visualization**
    - Typically chose k =2 or k = 3
    - Because we can plot these values!
- One thing often done wrong regarding PCA
    - A bad use of PCA: Use it to prevent over-fitting
        - Reasoning
            - If we have $x^i$ we have n features, $z^i$ has k features which can be lower
            - If we *only* have k features then maybe we're less likely to over fit...
        - This doesn't work
            - BAD APPLICATION
            - Might work OK, but not a good way to address over fitting
            - Better to use regularization
        - PCA throws away some data without knowing what the values it's losing
            - Probably OK if you're keeping most of the data
            - But if you're throwing away some crucial data bad
            - So you have to go to like 95-99% variance retained
                - So here regularization will give you AT LEAST as good a way to solve over fitting
- A second PCA myth
    - Used for compression or visualization - good
    - Sometimes used
        - Design ML system with PCA from the outset
            - But, what if you did the whole thing without PCA
        - See how a system performs without PCA
            - ONLY if you have a reason to believe PCA will help should you then add PCA
        - PCA is easy enough to add on as a processing step
            - Try without first!

# 15: Anomaly Detection

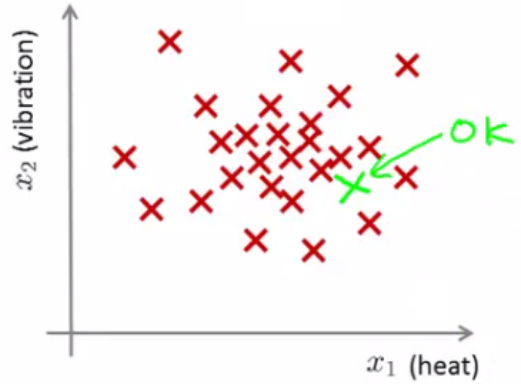


## Anomaly detection - problem motivation

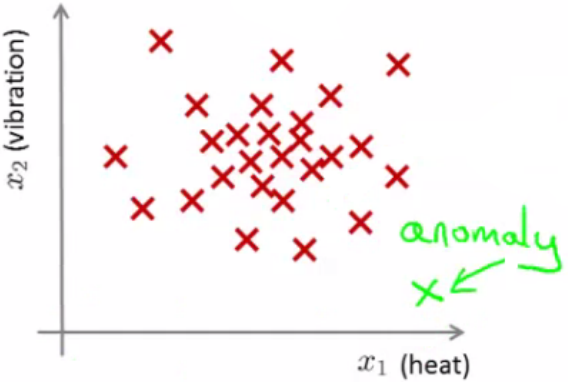
- Anomaly detection is a reasonably commonly used type of machine learning application
  - Can be thought of as a solution to an unsupervised learning problem
  - But, has aspects of supervised learning
- What is anomaly detection?
  - Imagine you're an aircraft engine manufacturer
  - As engines roll off your assembly line you're doing QA
    - Measure some features from engines (e.g. heat generated and vibration)
  - You now have a dataset of $x^1$ to $x^m$ (i.e. *m* engines were tested)
  - Say we plot that dataset




  - Next day you have a new engine
    - An anomaly detection method is used to see if the new engine is anomalous (when compared to the previous engines)
  - If the new engine looks like this;



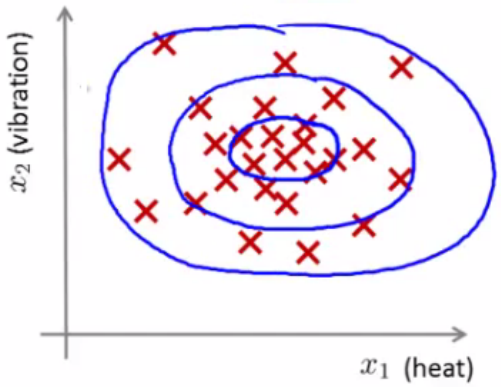

    - Probably OK - looks like the ones we've seen before
  - But if the engine looks like this




    - Uh oh! - this looks like an **anomalous data-point**

- More formally
  - We have a dataset which contains **normal** (data)
    - How we ensure they're normal is up to us
    - In reality it's OK if there are a few which aren't actually normal
  - Using that dataset as a reference point we can see if other examples are **anomalous**
- How do we do this?
  - First, using our training dataset we build a model

        - We can access this model using **p(x)**
            - This asks, "What is the probability that example x is normal"
    - Having built a model
        - if $p(x_{test}) < \varepsilon$ --> flag this as an anomaly
        - if $p(x_{test}) >= \varepsilon$ --> this is OK
        - $\varepsilon$ is some threshold probability value which we define, depending on how sure we need/want to be
    - We expect our model to (graphically) look something like this;




        - i.e. this would be our model if we had 2D data

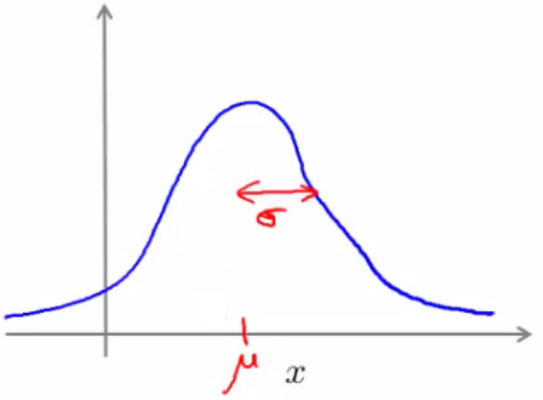
**Applications**

- Fraud detection
    - Users have activity associated with them, such as
        - Length on time on-line
        - Location of login
        - Spending frequency
    - Using this data we can build a model of what normal users' activity is like
    - What is the probability of "normal" behavior?
    - Identify unusual users by sending their data through the model
        - Flag up anything that looks a bit weird
        - Automatically block cards/transactions
- Manufacturing
    - Already spoke about aircraft engine example
- Monitoring computers in data center
    - If you have many machines in a cluster
    - Computer features of machine
        - $x_1$ = memory use
        - $x_2$ = number of disk accesses/sec
        - $x_3$ = CPU load
    - In addition to the measurable features you can also define your own complex features
        - $x_4$ = CPU load/network traffic
    - If you see an anomalous machine
        - Maybe about to fail
        - Look at replacing bits from it

# The Gaussian distribution (optional)

- Also called the **normal distribution**
- Example
    - Say x (data set) is made up of real numbers
        - Mean is $\mu$
        - Variance is $\sigma^2$
            - $\sigma$ is also called the **standard deviation** - specifies the width of the Gaussian probability
        - The data has a Gaussian distribution
    - Then we can write this $\sim N(\mu,\sigma^2)$
        - $\sim$ means = is distributed as
        - $N$ (should really be "script" N (even curlier!) -> means normal distribution
        - $\mu$, $\sigma^2$ represent the mean and variance, respectively
            - These are the two parameters a Gaussian means

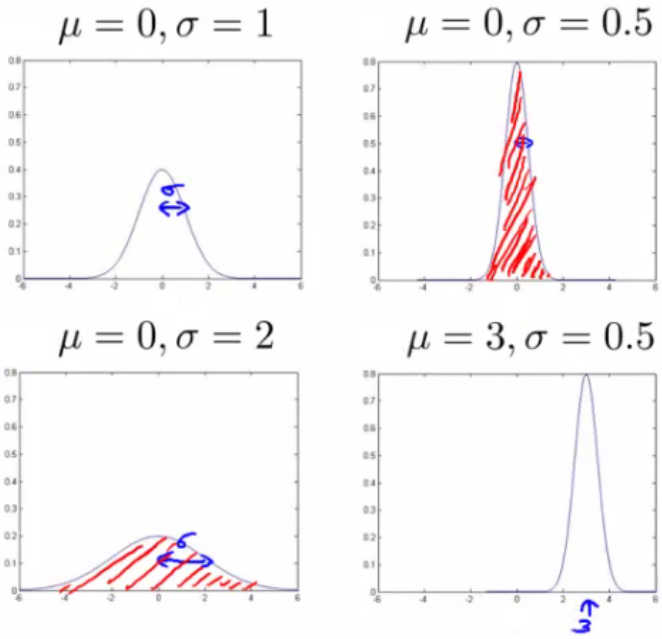
- Looks like this;




  - This specifies the probability of x taking a value
    - As you move away from μ
- Gaussian equation is
  - $P(x : \mu, \sigma^2)$ (probability of x, parameterized by the mean and squared variance)

$$= \frac{1}{\sqrt{2\pi}\sigma} exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- Some examples of Gaussians below
  - Area is always the same (must = 1)
  - But width changes as standard deviation changes

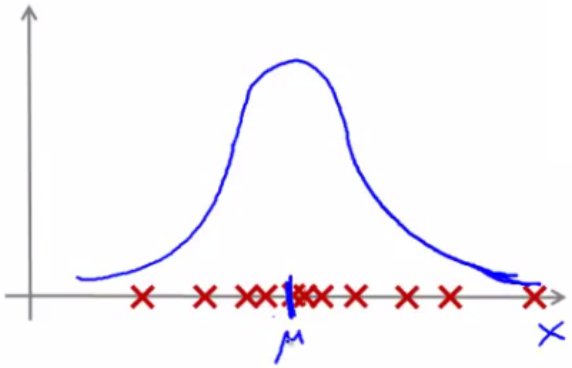



**Parameter estimation problem**

- What is it?
  - Say we have a data set of m examples
  - Give each example is a real number - we can plot the data on the x axis as shown below

  - Problem is - say you suspect these examples come from a Gaussian
    - Given the dataset can you estimate the distribution?

- Could be something like this




  - Seems like a reasonable fit - data seems like a higher probability of being in the central region, lower probability of being further away
- Estimating $\mu$ and $\sigma^2$
  - $\mu$ = average of examples
  - $\sigma^2$ = standard deviation squared

$$\sigma^2 = \frac{1}{m} \sum_{i=1}^{m} (x^{(i)} - \mu)^2$$

  - As a side comment
    - These parameters are the maximum likelihood estimation values for $\mu$ and $\sigma^2$
    - You can also do 1/(m) or 1/(m-1) doesn't make too much difference
      - Slightly different mathematical problems, but in practice it makes little difference

# Anomaly detection algorithm

- Unlabeled training set of m examples
  - Data = $\{x^1, x^2, ..., x^m\}$
    - Each example is an n-dimensional vector (i.e. a feature vector)
    - We have n features!
  - Model P(x) from the data set
    - What are high probability features and low probability features
    - x is a vector
    - So model p(x) as
      - $= p(x_1; \mu_1, \sigma_1^2) * p(x_2; \mu_2, \sigma_2^2) * ... p(x_n; \mu_n, \sigma_n^2)$
    - Multiply the probability of each features by each feature
      - We model each of the features by assuming each feature is distributed according to a Gaussian distribution
      - $p(x_i; \mu_i, \sigma_i^2)$
        - The probability of feature $x_i$ given $\mu_i$ and $\sigma_i^2$, using a Gaussian distribution
  - As a side comment
    - Turns out this equation makes an **independence assumption** for the features, although algorithm works if features are independent or not
      - Don't worry too much about this, although if you're features are tightly linked you should be able to do some dimensionality reduction anyway!
  - We can write this chain of multiplication more compactly as follows;

$$= \prod_{j=1}^{n} p(x_j; \mu_j, \sigma_j^2)$$

    - Capital PI ($\Pi$) is the product of a set of values
  - The problem of estimation this distribution is sometimes call the problem of **density estimation**

**Algorithm**

1. Choose features $x_i$ that you think might be indicative of anomalous examples.
2. Fit parameters $\mu_1, \ldots, \mu_n, \sigma_1^2, \ldots, \sigma_n^2$

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

$$\sigma_j^2 = \frac{1}{m}\sum_{i=1}^{m}(x_j^{(i)} - \mu_j)^2$$

3. Given new example $x$, compute $p(x)$:

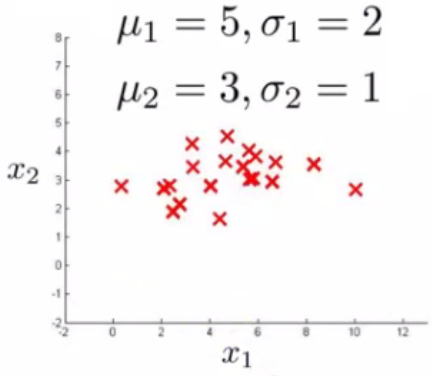
$$p(x) = \prod_{j=1}^{n} p(x_j; \mu_j, \sigma_j^2) = \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_j} \exp\left(-\frac{(x_j - \mu_j)^2}{2\sigma_j^2}\right)$$

Anomaly if $p(x) < \varepsilon$

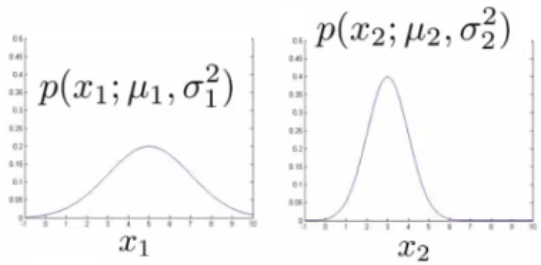
- **1 - Chose features**
  - Try to come up with features which might help identify something anomalous - may be unusually large or small values
  - More generally, chose features which describe the general properties
  - This is nothing unique to anomaly detection - it's just the idea of building a sensible feature vector
- **2 - Fit parameters**
  - Determine parameters for each of your examples $\mu_i$ and $\sigma_i^2$
    - Fit is a bit misleading, really should just be "Calculate parameters for 1 to n"
  - So you're calculating standard deviation and mean for each feature
  - You should of course used some vectorized implementation rather than a loop probably
- **3 - compute p(x)**
  - You compute the formula shown (i.e. the formula for the Gaussian probability)
  - If the number is very small, very low chance of it being "normal"

**Anomaly detection example**

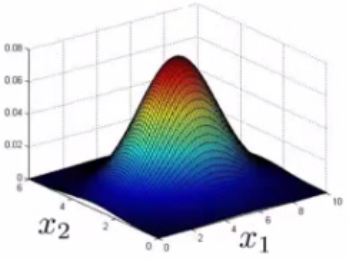
- $x_1$
  - Mean is about 5
  - Standard deviation looks to be about 2
- $x_2$
  - Mean is about 3
  - Standard deviation about 1
- So we have the following system




- If we plot the Gaussian for $x_1$ and $x_2$ we get something like this



- If you plot the product of these things you get a surface plot like this




  - With this surface plot, the height of the surface is the probability - p(x)
  - We can't always do surface plots, but for this example it's quite a nice way to show the probability of a 2D feature vector
- Check if a value is anomalous
  - Set epsilon as some value
  - Say we have two new data points new data-point has the values
    - $x^1_{test}$
    - $x^2_{test}$
  - We compute
    - $p(x^1_{test})$ = 0.436 >= epsilon (~40% chance it's normal)
      - Normal
    - $p(x^2_{test})$ = 0.0021 < epsilon (~0.2% chance it's normal)
      - Anomalous
  - What this is saying is if you look at the surface plot, all values above a certain height are normal, all the values below that threshold are probably anomalous

# Developing and evaluating and anomaly detection system

- Here talk about developing a system for anomaly detection
  - How to evaluate an algorithm
- Previously we spoke about the importance of real-number evaluation
  - Often need to make a lot of choices (e.g. features to use)
    - Easier to evaluate your algorithm if it returns a **single number** to show if changes you made improved or worsened an algorithm's performance
  - To develop an anomaly detection system quickly, would be helpful to have a way to evaluate your algorithm
- Assume we have some labeled data
  - So far we've been treating anomalous detection with unlabeled data
  - If you have labeled data allows evaluation
    - i.e. if you think something iss anomalous you can be sure if it is or not
- So, taking our engine example
  - You have some labeled data
    - Data for engines which were non-anomalous -> y = 0
    - Data for engines which were anomalous -> y = 1
  - Training set is the collection of normal examples
    - OK even if we have a few anomalous data examples
  - Next define
    - Cross validation set
    - Test set
    - For both assume you can include a few examples which have anomalous examples
  - Specific example
    - Engines
      - Have 10 000 good engines
        - OK even if a few bad ones are here...
        - LOTS of y = 0
      - 20 flawed engines
        - Typically when y = 1 have 2-50
    - Split into
      - Training set: 6000 good engines (y = 0)
      - CV set: 2000 good engines, 10 anomalous
      - Test set: 2000 good engines, 10 anomalous
      - Ratio is 3:1:1
    - Sometimes we see a different way of splitting
      - Take 6000 good in training
      - Same CV and test set (4000 good in each) different 10 anomalous,
      - Or even 20 anomalous (same ones)
      - This is bad practice - should use different data in CV and test set
  - Algorithm evaluation
    - Take trainings set { $x^1$, $x^2$, ..., $x^m$ }
      - Fit model p(x)

        - On cross validation and test set, test the example x
            - y = 1 if p(x) < epsilon (anomalous)
            - y = 0 if p(x) >= epsilon (normal)
        - Think of algorithm a trying to predict if something is anomalous
            - But you have a label so can check!
            - Makes it look like a supervised learning algorithm
- What's a good metric to use for evaluation
    - y = 0 is very common
        - So classification would be bad
    - Compute fraction of true positives/false positive/false negative/true negative
    - Compute precision/recall
    - Compute F1-score
- Earlier, also had **epsilon** (the threshold value)
    - Threshold to show when something is anomalous
    - If you have CV set you can see how varying epsilon effects various evaluation metrics
        - Then pick the value of epsilon which maximizes the score on your CV set
    - Evaluate algorithm using cross validation
    - Do final algorithm evaluation on the test set

# Anomaly detection vs. supervised learning

- If we have labeled data, we not use a supervised learning algorithm?
    - Here we'll try and understand when you should use supervised learning and when anomaly detection would be better

**Anomaly detection**

- **Very small number of positive examples**
    - Save positive examples just for CV and test set
    - Consider using an anomaly detection algorithm
    - Not enough data to "learn" positive examples
- **Have a very large number of negative examples**
    - Use these negative examples for p(x) fitting
    - Only need negative examples for this
- **Many "types" of anomalies**
    - Hard for an algorithm to learn from positive examples when anomalies may look nothing like one another
        - So anomaly detection doesn't know what they look like, but knows what they *don't* look like
    - When we looked at SPAM email,
        - Many types of SPAM
        - For the spam problem, usually enough positive examples
        - So this is why we usually think of SPAM as supervised learning
- Application and why they're anomaly detection
    - **Fraud detection**
        - Many ways you may do fraud
        - If you're a major on line retailer/very subject to attacks, sometimes might shift to supervised learning
    - **Manufacturing**
        - If you make HUGE volumes maybe have enough positive data -> make supervised
            - Means you make an assumption about the kinds of errors you're going to see
            - It's the unknown unknowns we don't like!
    - **Monitoring machines in data**

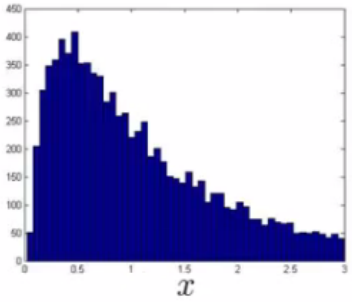
**Supervised learning**

- **Reasonably large number of positive and negative examples**
- Have enough positive examples to give your algorithm the opportunity to see what they look like
    - If you expect anomalies to look anomalous in the same way
- Application
    - Email/SPAM classification
    - Weather prediction
    - Cancer classification

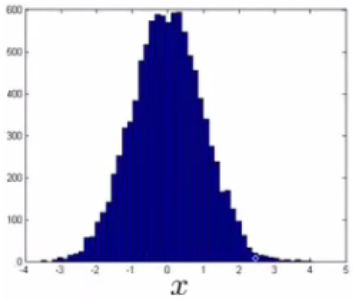
# Choosing features to use

- One of the things which has a huge effect is which features are used
- **Non-Gaussian features**
    - Plot a histogram of data to check it has a Gaussian description - nice sanity check
        - Often still works if data is non-Gaussian
        - Use **hist** command to plot histogram

- Non-Gaussian data might look like this



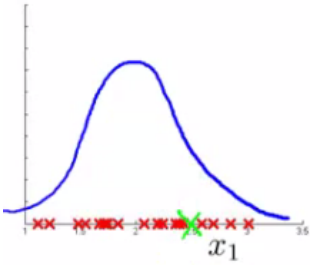

- Can play with different transformations of the data to make it look more Gaussian
- Might take a log transformation of the data
  - i.e. if you have some feature $x_1$, replace it with $\log(x_1)$




    - This looks much more Gaussian
  - Or do $\log(x_1+c)$
    - Play with c to make it look as Gaussian as possible
  - Or do $x^{1/2}$
  - Or do $x^{1/3}$

**Error analysis for anomaly detection**

- Good way of coming up with features
- Like supervised learning error analysis procedure
  - Run algorithm on CV set
  - See which one it got wrong
  - Develop new features based on trying to understand *why* the algorithm got those examples wrong
- Example
  - p(x) large for normal, p(x) small for abnormal
  - e.g.

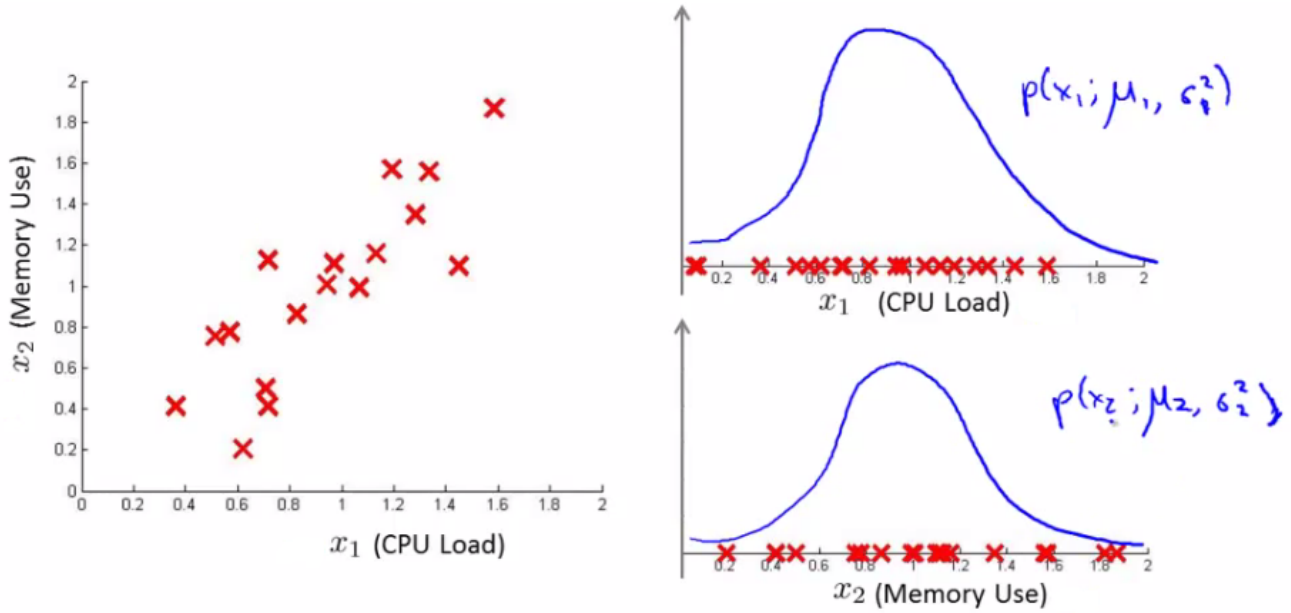



  - Here we have one dimension, and our anomalous value is sort of buried in it (in green - Gaussian superimposed in blue)
    - Look at data - see what went wrong
    - Can looking at that example help develop a new feature (x2) which can help distinguish further anomalous
- Example - data center monitoring
  - Features
    - $x_1$ = memory use
    - $x_2$ = number of disk access/sec
    - $x_3$ = CPU load
    - $x_4$ = network traffic
  - We suspect CPU load and network traffic grow linearly with one another
    - If server is serving many users, CPU is high and network is high
    - Fail case is infinite loop, so CPU load grows but network traffic is low
      - New feature - CPU load/network traffic
      - May need to do feature scaling

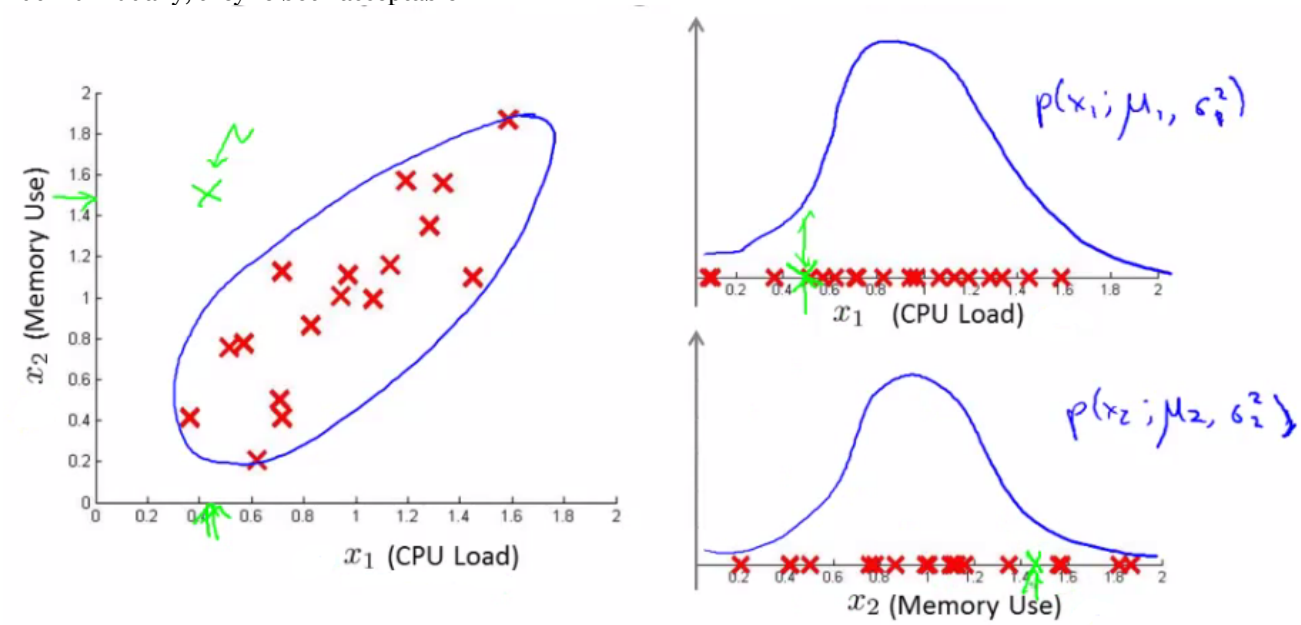
# Multivariate Gaussian distribution

- Is a slightly different technique which can sometimes catch some anomalies which non-multivariate Gaussian distribution anomaly detection fails to

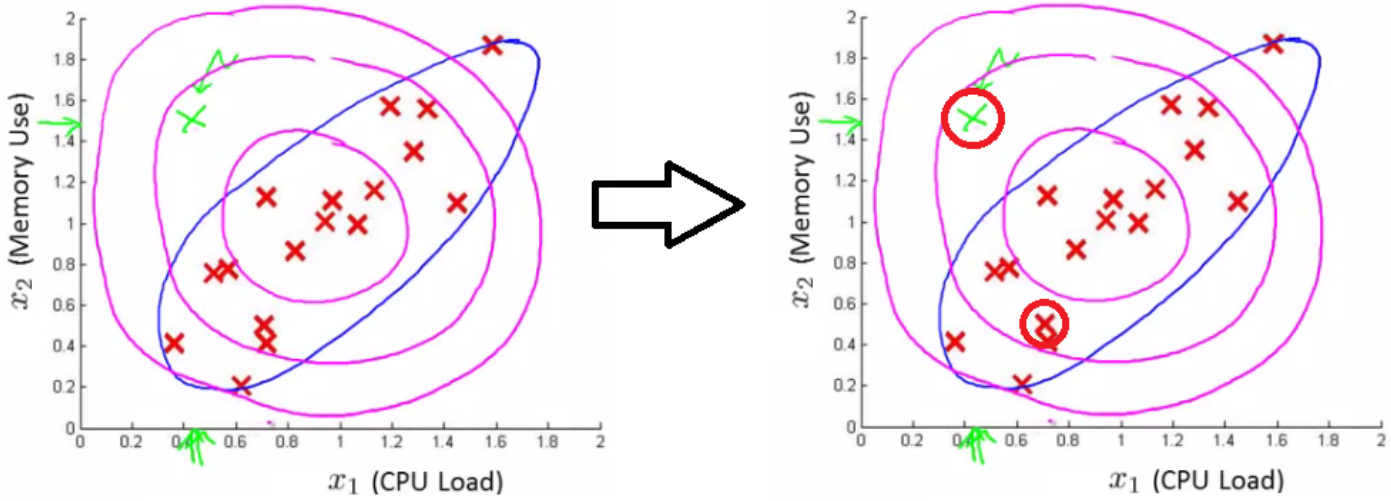
- Unlabeled data looks like this




- Say you can fit a Gaussian distribution to CPU load and memory use
- Lets say in the test set we have an example which looks like an anomaly (e.g. $x_1 = 0.4$, $x_2 = 1.5$)
  - Looks like most of data lies in a region far away from this example
    - Here memory use is high and CPU load is low (if we plot $x_1$ vs. $x_2$ our green example looks miles away from the others)
- Problem is, if we look at each feature individually they may fall within acceptable limits - the issue is we know we shouldn't don't get those kinds of values **together**
  - But individually, they're both acceptable




- This is because our function makes probability prediction in concentric circles around the the means of both




  - Probability of the two red circled examples is basically the same, even though we can clearly see the green one as an outlier

        - Doesn't understand the meaning

### Multivariate Gaussian distribution model

- To get around this we develop the **multivariate Gaussian distribution**
  - Model p(x) all in one go, instead of each feature separately
    - What are the parameters for this new model?
      - μ - which is an *n* dimensional vector (where n is number of features)
      - Σ - which is an [n x n] matrix - the **covariance matrix**

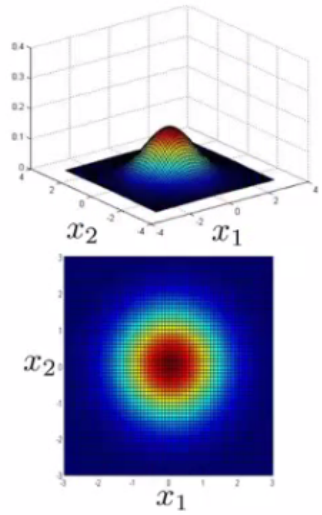
- For the sake of completeness, the formula for the multivariate Gaussian distribution is as follows

$$p(x;\mu,\Sigma) = \frac{1}{(2\pi)^{n/2}\,|\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

  - NB don't memorize this - you can always look it up
  - What does this mean?
    - $|\Sigma|$ = absolute value of Σ (determinant of sigma)
      - This is a mathematic function of a matrix
      - You can compute it in MATLAB using `det(sigma)`
- More importantly, what does this p(x) look like?
  - 2D example

$$\mu = \begin{bmatrix}0\\0\end{bmatrix} \Sigma = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$$

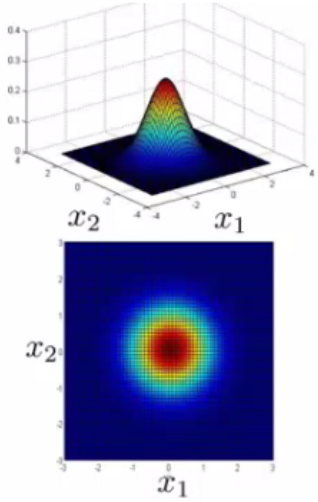
    - Sigma is sometimes call the identity matrix



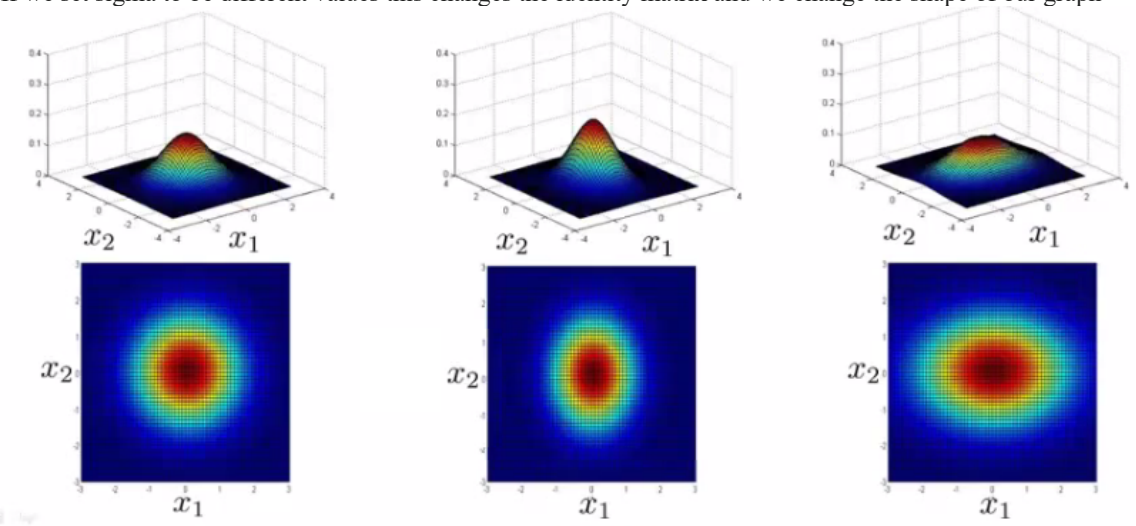

    - p(x) looks like this
      - For inputs of $x_1$ and $x_2$ the height of the surface gives the value of p(x)
  - What happens if we change Sigma?

$$\mu = \begin{bmatrix}0\\0\end{bmatrix} \Sigma = \begin{bmatrix}0.6 & 0\\0 & 0.6\end{bmatrix}$$

  - So now we change the plot to

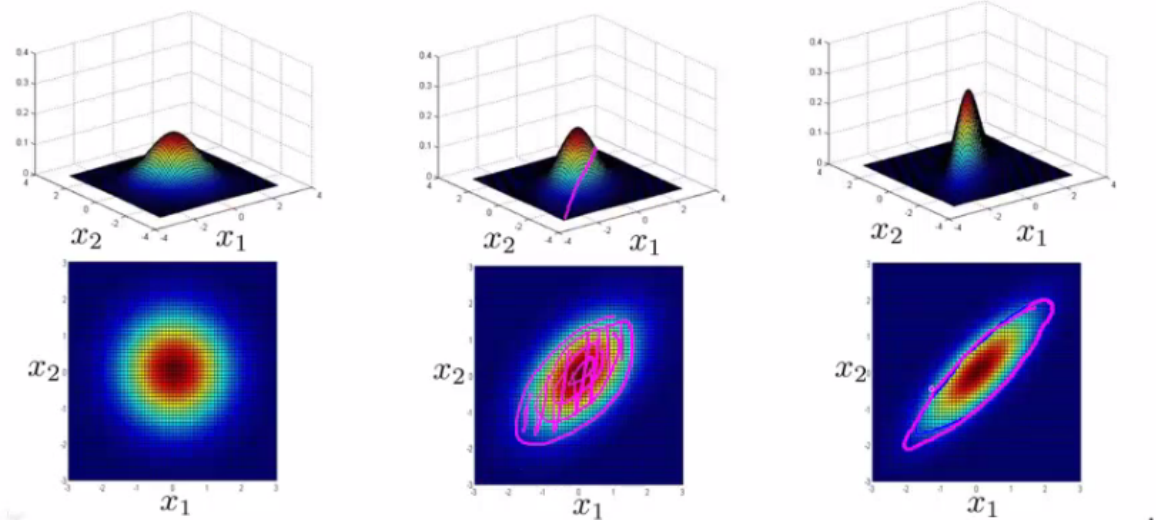


        - Now the width of the bump decreases and the height increases
    - If we set sigma to be different values this changes the identity matrix and we change the shape of our graph




    - Using these values we can, therefore, define the shape of this to better fit the data, rather than assuming symmetry in every dimension
- One of the cool things is you can use it to model correlation between data
    - If you start to change the off-diagonal values in the covariance matrix you can control how well the various dimensions correlation

$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix} \qquad \mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$




        - So we see here the final example gives a very tall thin distribution, shows a strong positive correlation
        - We can also make the off-diagonal values negative to show a negative correlation
- Hopefully this shows an example of the kinds of distribution you can get by varying sigma
    - We can, of course, also move the mean (μ) which varies the peak of the distribution

## Applying multivariate Gaussian distribution to anomaly detection

- Saw some examples of the kinds of distributions you can model
    - Now let's take those ideas and look at applying them to different anomaly detection algorithms
- As mentioned, multivariate Gaussian modeling uses the following equation;

$$p(x;\mu,\Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

- Which comes with the parameters μ and Σ
    - Where
        - μ - the mean (n-dimenisonal vector)
        - Σ - covariance matrix ([nxn] matrix)
- Parameter fitting/estimation problem
    - If you have a set of examples
        - $\{x^1, x^2, ..., x^m\}$
    - The formula for estimating the parameters is

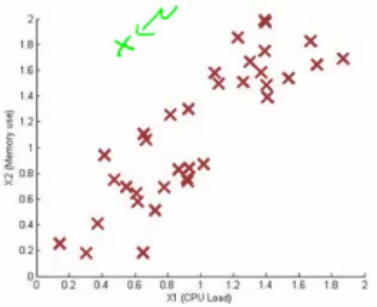
$$\mu = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$$

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

- Using these two formulas you get the parameters

**Anomaly detection algorithm with multivariate Gaussian distribution**

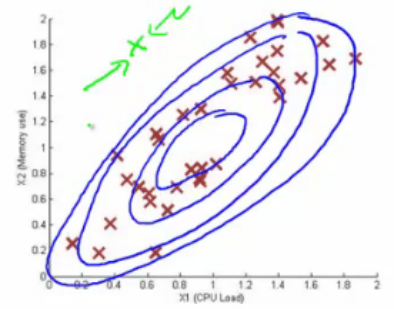
- **1)** Fit model - take data set and calculate μ and Σ using the formula above
- **2)** We're next given a new example ($x_{test}$) - see below




  - For it compute p(x) using the following formula for multivariate distribution

$$p(x) = \frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

- **3)** Compare the value with ε (threshold probability value)
  - if $p(x_{test}) < \varepsilon$ --> flag this as an anomaly
  - if $p(x_{test}) >= \varepsilon$ --> this is OK
- If you fit a multivariate Gaussian model to our data we build something like this




- Which means it's likely to identify the green value as anomalous
- Finally, we should mention how multivariate Gaussian relates to our original simple Gaussian model (where each feature is looked at individually)
  - Original model corresponds to multivariate Gaussian where the Gaussians' contours are axis aligned
  - i.e. the normal Gaussian model is a special case of multivariate Gaussian distribution
    - This can be shown mathematically
    - Has this constraint that the covariance matrix sigma as ZEROs on the non-diagonal values

$$p(x;\mu,\Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}}|\Sigma|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

where $\Sigma = \begin{bmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & & \ddots \\ & & & \sigma_n^2 \end{bmatrix}$

    - If you plug your variance values into the covariance matrix the models are actually identical

**Original model vs. Multivariate Gaussian**

<u>Original Gaussian model</u>

- Probably used more often
- There is a need to manually create features to capture anomalies where $x_1$ and $x_2$ take unusual combinations of values
  - So **need to make extra features**
  - Might not be obvious what they should be
    - This is always a risk - where you're using your own expectation of a problem to "predict" future anomalies
    - Typically, the things that catch you out aren't going to be the things you though of
      - If you thought of them they'd probably be avoided in the first place
    - Obviously this is a bigger issue, and one which may or may not be relevant depending on your problem space

- Much **cheaper computationally**
- **Scales much better** to very large feature vectors
  - Even if n = 100 000 the original model works fine
- **Works well even with a small training set**
  - e.g. 50, 100
- Because of these factors it's used more often because it really represents a optimized but axis-symmetric specialization of the general model

**Multivariate Gaussian model**

- Used less frequently
- **Can capture feature correlation**
  - So no need to create extra values
- **Less computationally efficient**
  - Must compute inverse of matrix which is [n x n]
  - So lots of features is bad - makes this calculation very expensive
  - So if n = 100 000 not very good
- **Needs for m > n**
  - i.e. number of examples must be greater than number of features
  - If this is not true then we have a singular matrix (non-invertible)
  - So should be used only in m >> n
- If you find the matrix is non-invertible, could be for one of two main reasons
  - m < n
    - So use original simple model
  - Redundant features (i.e. linearly dependent)
    - i.e. two features that are the same
    - If this is the case you could use PCA or sanity check your data