

Coursera- Machine Learning
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Summary

Supervised learning

- linear regression, logistic regression, neural network, SVMs

Unsupervised learning

- k-means, PCA, Anomaly detection

Special applications/special topics

- Recommender systems, large scale machine learning

Advice for building a machine learning system

- bias/variance, regularization, deciding what to work next, evaluation of a learning algorithm, learning curves, error analysis, ceiling analysis

Week 1

Intro

Definition of ML

- A program learns from experience (E) w.r.t task(T) and performance measure (P) if its performance on T improves with more E.
- With supervised learning, we know what our answers are as a relation of input and output. But with unsupervised learning, we have little idea about the result.

Cost function

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$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

our goal is to minimize the cost function, which is calculated as square error

$$\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$$

- where the error function is defined as

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

Linear regression

- Repeat until converge{ $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$ for $j = 0, 1$ }
- Note that the update is simultaneous :

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$$\text{temp}_0 := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$\text{temp}_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

$$\theta_0 := \text{temp}_0$$

$$\theta_1 := \text{temp}_1$$

- if we compute the derivative we get Repeat until converge{

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x_i) - y_i)$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m ((h_{\theta}(x_i) - y_i)x_i)$$

}

- α is the learning rate.
- we use linear regression algorithm to updates the parameters until we arrive at the minimal cost.

Week 2

Multi-feature linear regression

- Hypothesis

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \dots \theta_n x_n$$

- convenience $\forall x, x_0 = 1$, so that $h_{\theta} = \sum_{i=0}^n \theta_i x_i$

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$$x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1} \text{ and that } \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$$

- Hypothesis can be represented as

$$h_{\theta}(x) = \theta^T x \text{ or } \langle \theta, x \rangle$$

- The parameter we're estimating here is θ

- Cost function

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^m ((h_{\theta})x^{(i)} - y^{(i)})^2$$

- Gradient descent

$$repeat\{\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})x_j^{(i)}, \text{simultaneously update } \theta_0 \dots \theta_j\}$$

- When working with gradient descent in practice, we should... consider

- Feature scaling:

Make sure features are in a similar scale, so that each values are roughly between $[-3, 3]$

- Mean normalization: Replace all x_i (except for x_0) with $x_i - \mu_i$ so that the mean is roughly 0.

$$x_i \leftarrow \frac{x_i - \mu_i}{s_i}$$

- Note that J should always decrease w.r.t to the number of iteration. If it ever increases, that means our α , the step param, is too large. We would want to decrease α .

- Pick ϵ for the convergence threshold value.
- Tip: in order to choose α , try a range of values. Example: choosing based on a logarithmic scale:

$$0.001, 0.003, 0.01, 0.03, \dots$$

feature & polynomial regression

- We can combine multiple features into one and change the behaviour of the hypothesis.
- For example we can combine x_1, x_2 into a polynomial term by defining that $x_3 = x_1 * x_2$.
- polynomial regression, instead of linear, we make it quadratic or cubic to tune the hypothesis

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2^2 + \theta_3 \sqrt{x}$$

Keep in mind that feature scaling is still very important.

Normal equation: computing parameters analytically

- Define X as the design matrix. That is

$$\text{if } x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix} \text{ then we have } X = \begin{bmatrix} - & (x^{(1)})^T & - \\ - & (x^{(2)})^T & - \\ & \vdots & \\ - & (x^{(n)})^T & - \end{bmatrix}$$

- Optimum θ given by $\theta = (X^T X)^{-1} X^T y$
- With normal equation, you don't need feature scaling.

Gradient descent:

α needs to be chosen

needs many iterations

works well even when n is large

Normal equation:

no need to choose α

no iterations needed

computing $(X^T X)^{-1}$ takes $O(n^3)$

performs slow with large n ($n \geq 10,000$)

- Note: what if $X^T X$ is non-invertible? Then we use the *pinv* to generate the pseudo-inverse.

vectorization helps to compute vectors faster.

Week 3

Binary classification problems

- each element y belongs to negative class (0) or positive class (1).

Logistic regression

- We want $0 \leq h_\theta(x) \leq 1$
 $h_\theta(x) = g(\theta^T x)$ where g is the sigmoid function
 $g(z) = \frac{1}{1+e^{-z}}$

decision boundary

- The decision boundary is the line that separates area where $y = 0$ or $y = 1$.
- Note that

$$h_\theta(x) \geq 0.5 \iff \theta^T X \geq 0 \rightarrow y = 1$$

$$h_\theta(x) < 0.5 \iff \theta^T X < 0 \rightarrow y = 0$$

- we can also work with non-linear decision boundaries

Logistic regression model

- The training set will be $\{((x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)}))\}$
There are m examples, and for $\forall x, x \in \mathbb{R}^{n+1}$, $x_0 = 1$, $y \in \{0, 1\}$
 $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$
- We realize that lin.reg. will not give you a convex function but we want a convex function. This brings us to construct a good cost function.

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$$\text{cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

- For example if $y = 1$ then if $x = 1$ we have cost=0. And as hypothesis approach 0, cost approaches ∞ so we're penalized. Similar with the other situation.
- This gives us a convex and local optimum free function.
- The uncompressed cost function is:

$$\text{cost}(h_\theta(x), y) = -y \log(h_\theta(x)) - (1 - y) \log(1 - h_\theta(x))$$

- The total cost function J :

$$j(\theta) = \frac{1}{m} \sum_{i=1}^m \text{cost}(h_{\theta}(x), y)$$

- The gradient descent algorithm is essentially the same but referring to a different hypothesis which is $h_{\theta}(x)$ that now refers to the sigmoid function

The vectorized implementation

- $h = g(X\theta)$, which computes the quantity $h_{\theta}(x^{(i)})$
- $J(\theta) = \frac{1}{m}(-y^T \log(h) - (1 - y)^T \log(1 - h))$

Gradient descent

- Idea is to re-arrange the vectors until it's easier to type into matlab.
- Reminder that the matrix X looks like this:

$$X = \begin{bmatrix} - & (x^{(1)})^T & - \\ - & (x^{(2)})^T & - \\ & \vdots & \\ - & (x^{(m)})^T & - \end{bmatrix}$$

- X is a $m \times n$ matrix (ignoring the extra leftmost column of 1s). θ is a $n \times 1$ vector, which makes $X^T\theta$ a $m \times 1$ vector which yields the answer.

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$$\theta := \theta - \frac{\alpha}{m} \sum_{i=1}^m [(h_{\theta}(x^{(i)}) - y^{(i)})x_j^{(i)}]$$

note that the x is a column vector.

- the vectorized version is:

$$\theta := \theta - \frac{\alpha}{m} X^T (g(X\theta) - \bar{y})$$

- Advanced optimization: Given the cost function $J(\theta)$ and gradient $\frac{\partial}{\partial \theta_j} J(\theta)$ we can compute $\min_{\theta} J(\theta)$.
- These following algorithms are more complex but compute θ at a faster rate, and there is no need to compute α .

- Conjugate gradient, BFGS, L-BFGS
- Use the function "fminunc()"

Logistic optimization for multiple classes

- Multiple classification is the situation when $y = \{0, \dots, n\}$. i.e. we have different classes of outcomes. Our strategy is to assign one class as 'positive' and the rest of classes as 'the rest'.
- $y \in \{0, 1, 2, \dots, n\}$
- $h_{\theta}^{(0)}(x) = P(y = 0 \mid x; \theta)$
- $h_{\theta}^{(1)}(x) = P(y = 1 \mid x; \theta)$
- \vdots
- $h_{\theta}^{(n)}(x) = P(y = n \mid x; \theta)$
- The prediction is $\max_i h_{\theta}^{(i)}(x)$

The problem of over-fitting

- Underfitting: the hypothesis function fits too poorly onto the trend of the data, the function is either too simple or accounting too little features.
- Overfitting: the hypothesis function is not generalized enough. It fits well with given data but presents unnecessary corners/ angles.
- To resolve overfitting, we can either 1) reduce the number of features, i.e. have an algorithm that ditches unimportant features. Or 2) apply regularization to reduce magnitude of some features.

Cost function with regularization

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

- We want a big λ so that bumps up and forces θ_j to be small as we penalize bit θ_j .

Gradient descent

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$$\begin{aligned} \text{repeat } \{ \theta_0 &:= \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)} \text{ and} \\ \theta_j &:= \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right] \\ \text{for } j &= \{1, \dots, n\} \end{aligned}$$

- or we can equivalently write this in one equation:

$$\theta_j := \theta_j \left(1 - \alpha \frac{\lambda}{m} - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} \right)$$

Normal Equation

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$$\theta = (X^T X + \lambda L)^{-1} X^T y$$

- where L is the same as $I \in M_n^{(n+1) \times (n+1)}$ with the first 1 replaced with 0. Note that if $m < n$ then $X^T X$ is non-invertible but adding L makes it invertible. Hence regularization also solves non-invertability.

Regularized logistic equation

(note that advanced optimization method me mentioned earlier also works here)

- Regularized cost function for logistic regression is:

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

- the last term is newly added for the regularization

- Gradient descent is exactly the same

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$$\begin{aligned} \text{repeat } \{ \theta_0 &:= \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)} \text{ and} \\ \theta_j &:= \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right] \\ \text{for } j &= \{1, \dots, n\} \end{aligned}$$

Advanced functions (regularization)

- $Jval$ does not change while the gradients do change.

- Gradient 1(index 0):

$$\frac{1}{m} \sum_{i=1}^m (h_{\theta}(X^{(i)}) - y^{(i)}) x_0^{(i)}$$

- Gradient 2(index 1, 2, ... n)

$$\left(\frac{1}{m} \sum_{i=1}^m (h_{\theta}(X^{(i)}) - y^{(i)}) x_0^{(i)} \right) + \frac{\lambda}{m} \theta_j$$

note that the last term is a newly added item.

Week 4

Neural Networks model representation

- We use matrices and vectors to model neurons and layers. [I'm too lazy to use tikz to draw it]
- Neural network is consisted of multiple layers. There is an input-layer, lots of hidden layer in the middle and the output layer wich is one node.
- $a_i^{(j)}$ = "activation" of unit i in layer j .
- $\Theta^{(j)}$ = matrix of weights controlling function mapping from layer j to layer $j + 1$.
- Vec representation

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \rightarrow \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \\ a_3^{(2)} \end{bmatrix} \rightarrow h_{\Theta}(x)$$

- Layer 1 to layer 2:

$$\begin{aligned} a_1^{(2)} &= g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3) \\ a_2^{(2)} &= g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3) \\ a_3^{(2)} &= g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3) \end{aligned}$$

- Layer 2 to layer 3:

$$h_{\Theta}(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

- What is the dimension of Θ ?
- Note that each layer has its own matrix of weights. If network has S_j layers in level j and S_{j+1} layers in level $j + 1$ then $\Theta^{(j)}$ has dimensions $S_{j+1} \times (S_j + 1)$ where the extra 1 comes from the bias node.
- the intuition is that NN allows nodes in its hidden layer to 'learn' its own features.

Vectorization of Computation

- $a_1^{(2)} = g(z_1^{(2)})$

- $a_2^{(2)} = g(z_2^{(2)})$
- $a_3^{(2)} = g(z_3^{(2)})$
- For layer j , node k , z is $z_k^{(j)} = \Theta_{k0}^{(j-1)}x_0 + \Theta_{k1}^{(j-1)}x_1 + \dots + \Theta_{kn}^{(j-1)}x_n$

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$$\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} z^{(j)} \begin{bmatrix} z_1^{(j)} \\ z_2^{(j)} \\ \vdots \\ z_n^{(j)} \end{bmatrix} \rightarrow h_{\Theta}(x)$$

- note that

$$z^{(j)} = \Theta^{(j-1)}a^{(j-1)}$$

since dimensions of Θ is $S - j \times n + 1$ and that dimensions of a is $n + 1 \times 1$.

- We add the bias unit to layer j after computing $a^{(j)}$ i.e. $a_0^{(j)} = 1$.
- In order to compute the final hypothesis, we compute the final z vector, where the last matrix of Θ only has 1 row, which multiplied by a column will result in a real number.

$$h_{\Theta}(x) = a^{(j+1)} = g(z^{(j+1)})$$

- Multi-class classification- we still use the one-vs all method. We set $h_{\Theta}(x) \in \mathbb{R}^4$ if there are 4 classes.

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$$h_{\Theta}(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

with different input x . It returns one of the standard vectors e_i s given a particular input.

Week 5

Our goal is to learn how to train NNs.

The cost function for NN

- L : is the total number of layers in the NN
- S_l : is the number of units not counting the bias unit in layer l
- k : is the number of output unit/ classes
- The cost function is:

$$J(\Theta) = -\frac{1}{m} \sum_{i=1}^m \sum_{k=1}^m [y_k^{(i)} \log((h_{\Theta}(x^{(i)}))_k) + (1 - y_k^{(i)}) (\log(1 - h_{\Theta}(x^{(i)}))_k)] + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} (\Theta_{j,i}^{(l)})^2$$

The back propagation algorithm

- The goal is to compute $\min_{\Theta} J(\Theta)$.
- look at the partial derivative of $J(\Theta)$, which is

$$\frac{\partial}{\partial \Theta_{i,j}^{(l)}} J(\Theta)$$

, The back propagation algorithm works as follows:

- given the training sets $\{(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})\}$
- we set $\Delta_{i,j}^{(l)} := 0 \forall i, j$
- For training exmples $t = 1 \sim m$:
 - 1. Set $a^{(1)} := x^{(t)}$
 - 2. Perform forward propagation to compute $a^{(l)}$ for $l = 1, 2, \dots, L$
(i.e. set up z (intermediate value) and use $g(z)$ to calculate next layers, so on and so on.
 - 3. $\delta^{(L)} = a^{(L)} - y^{(t)}$

- 4. compute $\delta^{(L-1)}, \delta^{(L-2)}, \dots, \delta^{(2)}$ using

$$\delta^{(l)} = ((\Theta^{(l)})^T \delta^{(l+1)}) .* a^{(l)} .* (1 - a^{(l)})$$

where the first value is the calculated value and that the second value is derivative of g which is g' .

$$g'(z^{(l)}) = a^{(l)} .* (1 - a^{(l)})$$

Note: $.*$ means product form direct vector multiplication. i.e. resulting vector takes i^{th} value from the product of the two i^{th} values from the multiplicands.

- 5. $\Delta_{i,j}^{(l)} := \Delta_{i,j}^{(l)} + a_j^{(l)} \delta_j^{(l+1)}$
with vectorization we have $\Delta_{i,j}^{(l)} := \Delta_{i,j}^{(l)} + \delta_j^{(l+1)} (a_j^{(l)})^T$
- Hence the update is

$$D_{i,j}^{(l)} := \begin{cases} \frac{1}{m} \Delta_{i,j}^{(l)} + \lambda_{\Theta_{i,j}}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{m} \Delta_{i,j}^{(l)} & \text{if } j = 0 \end{cases}$$

- In here, D is the accumulator for the gradient where $\frac{\partial}{\partial \Theta_{i,j}^{(l)}} J(\Theta) = D_{i,j}^{(l)}$
- Very useful resources to read about:
”<http://neuralnetworksanddeeplearning.com/chap2.html>”
- Tips for implementation:
 1. For this part, the homework assignment did not ask you to implement these steps.
 2. Unrolling is basically changing a matrix into a single column vector, i.e. unrolling
 3. Gradient checking ensures bug-free implementation
 4. Initial theta is set randomly

Week 6

Evaluating a learning algorithm

- What are some ways to arrive at a better hypothesis?
More examples
more / less # of features
more / less values of λ
- To evaluate a hypothesis, we split the data into training set and the test sets. They usually have 70% and 30% respectively.
- Then we learn Θ , minimize $j_{train}(\Theta)$ using the training set. Next step we evaluate how good our hypothesis is by calculating the test set error with $J_{test}(\Theta)$.
- to compute the test set error for lin.reg., it is half of the square error, whereas for log.reg. it is the average of the *err* function where it is 1 if hypothesis is in the right range, 0 otherwise.

Model selection

- We can break down the data-set into three data-sets:

training set, cross validation set, and test set

taking up 60%, 20%, 20% respectively.
- We can test different degree of polynomial, evaluate their error functions.
 1. optimize params in Θ using training set for each degree.
 2. find the polynomial degree d that produce least error by cross validation set.
 3. estimate generalized error with test set.

Diagnosing bias, variance and regularization, learning curves

- Better explanation seen in the handwritten notes- it has graph examples.

debugging a learning algorithm

problem	try
high var	get more training data
high var	less features
high var	increase λ
high bias	get more features
high bias	add polynomial features
high bias	decrease λ

Note that small NN are computationally cheap but prone to underfitting.

Large NN are computationally expensive but prone to overfitting. Note that λ regularization can be use to fix this problem.

Error analysis

- Always implement a quick implementation, and use that to decide how to spend your time.
- Plot learning curves and use that to decide about your next steps. You can manually examine your errors or impementa metric that returns your performance.
- For skewed classes, for example one class has very large size and another has very little, we use another error metric that accounts true and false positives and negatives. (F scores)

Week 7

SVMs

- SVM for logistic regression works with different cost function, that is easier to compute for the computer. It allows a large margin classifier that draws the decision boundary that stays naturally far apart from the dataset. kernels take data as input and transform them into the required forms.
- When using a SVM, we can use nice libraries such as *liblinear* or *libsvm*. We need to choose kernel (linear kernel a.k.a. no-kernel or gaussian kernel) as well as parameter c .
- Other choices of kernel must satisfy Mercer's theorem so that it does not diverge.
- for multi-classification, we can use the built-in SVM package or the one-vs-all methods.

Week 8

Unsupervised learning

- The given input has no labels
- the algorithm finds clustering data, and it identifies structures. It can be used for identifying market segmentations, social network analysis, organize computer clusters, and galaxy formation/astronomical data analysis.

k-means algorithm

- This is used to identify clustering.
- Step 1. Initialize cluster centroids randomly
- Step 2. assign each point to centroids that is the closest
- Step 3. move the centroids, to new means of assigned points
- Step 4. repeat
- The input is:
 - k : the number of clusters.
 - Training set: $\{x^1 \dots x^m\}$ for each $x^i \in \mathbb{R}^k$
 - It can also be used for non-separating clusters, although it may not seem like an obvious pattern.

Optimization objectives

- $c^{(i)}$ is the index of cluster ($1 \sim k$) that $x^{(i)}$ is currently assigned to.
- u_k is the cluster centroid k .
- $u_c^{(i)}$ is the cluster centroid that $x^{(i)}$ is currently assigned to.
- Our objective is:

$$\min_{c, \mu} J(c^{(1)}, c^{(2)}, \dots, c^{(m)}, \mu_1, \dots, \mu_k)$$

where

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

Random initialize clustering centroid

- select $k < m$, randomly choose k training examples, and the μ_1, \dots, μ_k to these examples.
- To avoid bad clustering, we can initiate randomly many times, and compare the J and pick the one that has smallest cost to start with.

Pick # of clusters

- Plot # of clusters on x-axis and cost function on y-axis, and locate the "elbow" .
- Another method is to pick k from what you want to do with the result of learning.

Data compression

- reducing redundant data. For example, if we're to record dataset that forms one line then using 2-d structures to record this data is redundant.

visualization

- we choose the 2 or 3 of the features and plot them. This helps us to recognize the relationships between features.

PCA: Principle component analysis

- our goal is to find a surface of a lower dimension such that it has the smallest sum of distance from each point in the dataset to the projected point.
- Note that PCA is not lin.reg, because PCA minimizes the perpendicular distance (has nothing to do with the outcome y) where lin.reg predicts y by minimizing vertical distance.

The PCA algorithm

- The training set is $\{x^1, \dots, x^m\}$
- First, we must do pre-processing (or feature scaling, mean normalization)
- $u_j = \frac{1}{m} \sum_{i=1}^m x_j^{(i)}$, and replace each $x_j^{(i)}$ with $x_j - \mu_j$
- We then also scale the features i.e. $x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j}$
- Then, we compute the vector μ_i and projections/ new representations.
- We reduce the data from dim n to dim k . The covariance matrix is : $\Sigma : \frac{1}{m} \sum_{i=1}^n (x^{(i)})(x^{(i)})^T$

- The eigenvalues of Σ is $[U, S, V] = \text{svd}(\Sigma)$
- U will be a $n \times n$ matrix whose columns are u^1, \dots, u^m . i.e. the eigenvectors.

$$A = \begin{bmatrix} | & | & & | \\ \mu_1 & \mu_2 & \dots & \mu_m \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n \times m} \text{ where we choose the first } k \text{ as the } k \text{ dimensions}$$

so that

$$\mu_{\text{reduce}} = \begin{bmatrix} | & | & & | \\ \mu^1 & \mu^2 & \dots & \mu^k \\ | & | & & | \end{bmatrix} z^{(i)} = \mu_{\text{reduce}}^T x^{(i)}$$

Reconstruction from compressed representation

- $z = \mu_{\text{reduce}}^T * X$
- $X_{\text{approx}} = \mu_{\text{reduce}} * z$

Applying PCA

- How to choose k ?

$$\text{The average square projection error is} = \frac{1}{m} \sum_{i=1}^m \|x^{(i)} - x_{\text{approx}}^{(i)}\|^2$$

$$\text{total variance in data is} = \frac{1}{m} \sum_{i=1}^m \|x^{(i)}\|^2$$

- We choose k to be the smallest value such that

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

- That is, we need 99% of variance to be retained.
- For the algorithm implementation, $[U, S, V] = \text{svd}(\Sigma)$, where S is a diagonal matrix. Pick smallest k such that

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

How to use PCA to speed up learning algorithm

- When running PCA, we only run it on the training set.
- To speed it up, we have input $\{(x^1, y^1), \dots (x^m, y^m)\}$ for $\forall x \in \mathbb{R}^{10000}$. Then the extracted input is $\{z^1, z^2, \dots z^m \in \mathbb{R}^{1000}\}$
- Now we train $\{(z^1, y^1), \dots (z^m, y^m)\}$.

Summary of application of PCA

- Compression: reduce storage to store data, and speed up the learning algos.
- Visualization: use $k = 2$ or $k = 3$
- Note: don't use PCA to prevent overfitting, and we should use regularization instead.
- Note: when designing system, first try without PCA, and only use PCA is necessary.

Week 9

Anomaly detection

- Detects anomalously behaving data, by using Gaussian distribution
- Density estimation: training set = $\{x^1, \dots, x^m\} \forall x, x \in \mathbb{R}^n$
- $P(x) = \prod_{j=1}^n p(x_j; u_j, \theta_j^2)$

Anomaly detection algorithm

1. Choose features x_i that you think might be anomaly
2. fit params $u_1, \dots, u_n, \theta_1^2, \dots, \theta_n^2 \rightarrow u_j = \frac{1}{m} \sum x_j^{(i)}, \theta_j^2 = \frac{1}{m} \sum (x_j^{(i)} - u_j)^2$
3. given new example x , compute $p(x) = \prod_{j=1}^n p(x_j; u_j, \theta_j^2)$.

Developing and evaluating an anomaly detection system

- We use the training set, cross validation set, and the test set.
- To evaluate whether a training data is anomaly, we first fit the models using training and cv sets, where we pick a threshold value ϵ . If p returns greater than ϵ , it is normal, otherwise an anomaly.
- We use the cv set to find ϵ .
- Note that multivariate Gaussian distribution can detect abnormal relationships between features. It is more computationally expensive. To do so, we must have $m > n$ or else Σ is singular.

When should we use anomaly detection? When to use supervised learning?

- AD
Very small number of positive example, and large number of negative examples
there are many types of anomaly, that makes learning difficult
very possible to encounter anomaly in the future that we have never seen.
- SL
Large number of positive and negative examples
future anomaly may look like previous ones
there is enough positive examples for the algorithm to learn.

Recommender systems

- give recommendation to subscribers to a service
- this is a high-priority to many companies i.e. Predicting movies for Netflix.
- Collaborative filtering algorithms
- Let x be the features for users and the θ be the features for movies.
- 1. Initialize $x^1, \dots, x^{nm}, \theta^1, \dots, \theta^{nu} \in \mathbb{R}^n$ to small values.
- 2. minimize $J(x^1, \dots, x^{nm}, \theta^1, \dots, \theta^{nu})$ using gradient descent or other advanced optimization algorithms. for example

$$x_k^i = x_k^i - \alpha \left(\sum_{j:r(i,j)=1} ((\theta^{(j)})^T x^{(i)} - y^{i,j}) \theta_k^{(i)} + \lambda x_k^{(i)} \right)$$

$$\theta_k^j = \theta_k^j - \alpha \left(\sum_{i:r(i,j)=1} ((\theta^{(j)})^T x^{(i)} - y^{i,j}) x_k^{(i)} + \lambda \theta_k^{(j)} \right)$$

- 3. For a user with parameters θ and a movie with (learned) features x , predict a star rating of $\theta^T x$.
The vectorized implementation is in video, "low rank matrix factorization".
- For newly registered users, we use mean normalization to predict entries with no previous data.