

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 update 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)

- J_{val} 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