

Machine Learning: Multivariate Linear Regression

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Multiple Features

- Notation usage
 - n - number of features
 - m - number of training examples
 - $x^{(i)}$ - input features of i th training example -> is a vector with dimension n
 - $x_j^{(i)}$ - number of feature j in i th training example
- Hypothesis is of the form $h_\theta(x) = \theta_0 + \theta_1 x_1 + \dots + \theta_n x_n$
 - Define $x_0 := 1$ as coefficient of θ_0
 - * Let $x = \begin{bmatrix} x_0 \\ \vdots \\ x_n \end{bmatrix}$ and $\theta = \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_n \end{bmatrix}$
 - * Both are in \mathbb{R}^{n+1}
 - Thus $h_\theta(x) = \theta^T x$ where θ is transposed to allow multiplication with matrix x

Gradient descent with multiple features

- Let θ be the $n + 1$ -dimensional parameter vector
- Perform $\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$
 - Simultaneous update of θ_j for $j = 0, \dots, n$

repeat until convergence:

$$\begin{aligned}\theta_0 &:= \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_0^{(i)} \\ \theta_1 &:= \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)} \\ \theta_2 &:= \theta_2 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_2^{(i)}\end{aligned}$$

Feature Scaling

- Make sure features are on similar scale or interval
 - Contours will become more like circles -> gradient descent is less complicated
- Get feature into approx. $-1 \leq x_i \leq 1$ range
- Mean normalization
 - Replace x_i with $x_i - \mu_i$ to make features have an approximately zero mean (except $x_0 = 1$)
- Thus formula for feature scaling with mean normalization is $x_i \rightarrow \frac{x_i - \mu_i}{s_i}$ where s_i can be range of values in training set or the std. dev

Learning rate

- Debugging gradient descent

- Plot $\min J(\theta)$ as gradient descent runs over # of iterations
 - Should show decrease as iterations progress
- Automatic convergence test
 - Ex: Declare convergence if $J(\theta)$ decreases by less than 10^{-3} in 1 iteration
- For sufficient small α $J(\theta)$ decreases on every iteration
 - If too small -> slow to converge

Features and Polynomial Regression

- Can define a feature in terms of others -> combining features
- Fitting polynomial model
 - Define each feature to be square, cubed, etc.
 - Apply regular linear Regression
 - Feature scaling is important -> exponential values increase scale

Normal Equation

- Method to solve for $\theta_0, \dots, \theta_n$ through derivative of J with respect to θ_j , set to 0, and minimization
- Construct a design matrix X that is of dimension $m \times (n + 1)$ and contains all of the training data
 - Each feature vector $x^{(i)} \in \mathbb{R}^{n+1}$ is transposed to constitute a row of X
- Construct vector y which contains the result/expected output and is m -dimensional
- Optimum θ is given by $\boxed{(X^T X)^{-1} X^T y}$
- Feature scaling not required
- Gradient descent comparison
 - Gradient descent -> need to choose α and needs many iterations
 - * Works well for a large n
 - Normal equation -> no need to choose α and don't need to iterate
 - * Slow if n is very large -> need to compute $(X^T X)^{-1}$
 - Inversion is $O(n^3)$
- $X^T X$ can be noninvertible
 - `pinv` works regardless of invertibility and `inv` will throw error in octave
 - Redundant features (i.e. linear dependence)
 - Too many features means $m \leq n$