

4. MULTIVARIATE LINEAR REGRESSION:

Multiple features (variables).

Size (feet ²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price (\$1000) y
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
...

$m = 47$

Notation:

- n = number of features $n = 4$
- $x^{(i)}$ = input (features) of i^{th} training example.
- $x_j^{(i)}$ = value of feature j in i^{th} training example.

$$x^{(2)} = \begin{bmatrix} 1416 \\ 3 \\ 2 \\ 40 \end{bmatrix} \in \mathbb{R}^4$$

$$x_3^{(2)} = 2$$

Hypothesis:

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

For convenience of notation, define $x_0 = 1$. ($x_0^{(i)} = 1$)

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

$$h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \dots + \theta_n x_n$$

$$= \theta^T x$$

θ^T is a $(n+1) \times 1$ matrix

Multivariate linear regression. ←

\mathbf{X} = features vector or design vector

Θ^T = transpose of Θ

Θ = parameter vector

m = the number of training examples

n = the number of features

$$h_{\theta}(x) = [\theta_0 \quad \theta_1 \quad \dots \quad \theta_n] \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} = \theta^T x$$

In order to develop intuition about this function, we can think about θ_0 as the basic price of a house, θ_1 as the price per square meter, θ_2 as the price per floor, etc. x_1 will be the number of square meters in the house, x_2 the number of floors, etc.

Cost function:

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

Gradient descent:

Repeat {

$$\rightarrow \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \dots, \theta_n) \quad \underline{J(\theta)}$$

(simultaneously update for every $j = 0, \dots, n$)

➤ In **linear regression** with **ONE VARIABLES**: $n=1$

➔ thus $n+1 = 2$ ➔ for Θ_0 and Θ_1

For **multiple variables**: $n > 1$

➤ New algorithm ($n \geq 1$):

Repeat {

$$\downarrow \frac{2}{2\theta_j} J(\theta)$$

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

(simultaneously update θ_j for
 $j = 0, \dots, n$)

}

$$x_0^{(i)} = 1$$

$$\rightarrow \underline{\theta_0} := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \underline{x_0^{(i)}}$$

$$\rightarrow \theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \underline{x_1^{(i)}}$$

$$\rightarrow \theta_2 := \theta_2 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_2^{(i)}$$

...

Feature Scaling

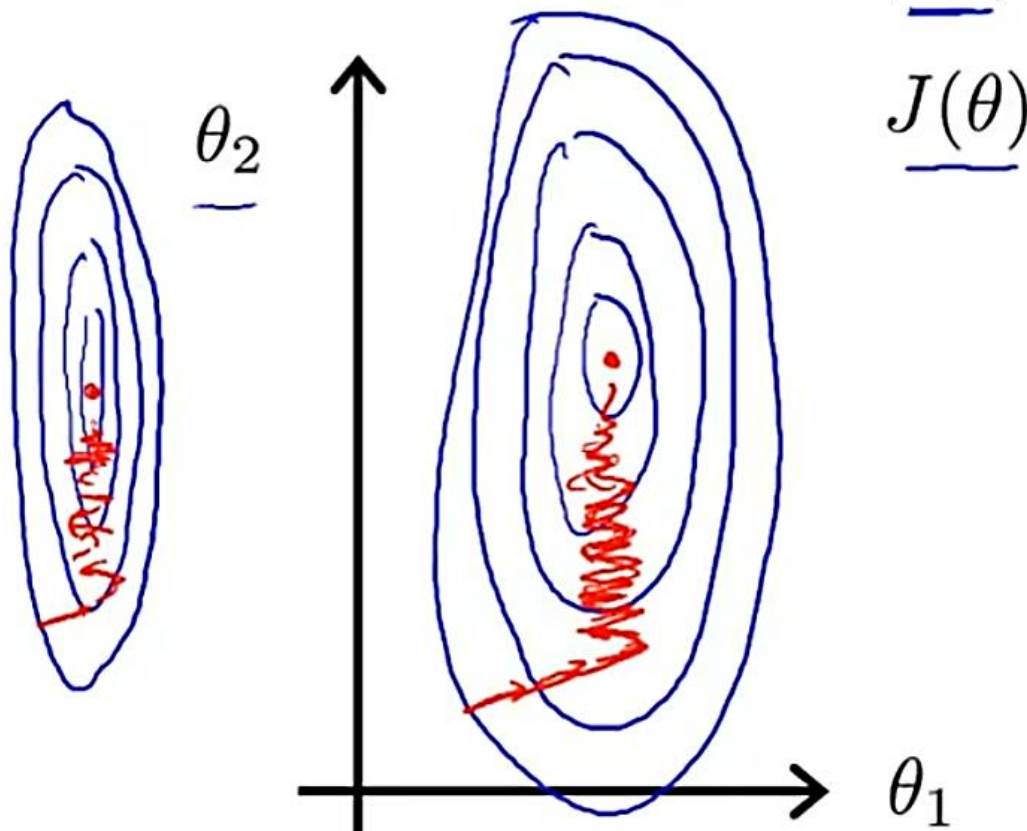
Idea: Make sure features are on a similar scale.

- Used when all input var. have different range of allowed values. This makes optimizing slower. Its tedious to find the local minima.

Example: if diff ranges are used the contours are quite **steep** type

E.g. $x_1 = \text{size (0-2000 feet}^2\text{)}$ ←

$x_2 = \text{number of bedrooms (1-5)}$ ←



- θ will descend quickly on small ranges and slowly on large ranges, and so will oscillate inefficiently down to the optimum when the variables are very uneven.

To solve this: we can change **scaling** of x_1 and x_2

This will make the contours more **balanced**.

This is done to bring approximate values of all x_i near a **same range**.

$$-1 \leq x_i \leq 1$$

-1 and 1 are not necessary for all x_i ...we can work with nearly equal ranges, like -3 to 3, etc... **comparable ranges**

- We can **speed up gradient descent** by having each of our input values in roughly the same range.

Ranges that would work:

$$0 \leq x_1 \leq 3 \quad \checkmark$$

$$-2 \leq x_2 \leq 0.5 \quad \checkmark$$

$$-3 \text{ to } 3$$

$$-\frac{1}{3} \text{ to } \frac{1}{3} \quad \checkmark$$

Ranges that won't work: if ranges are too large or too smaller than ± 1

$$-100 \leq x_3 \leq 100 \quad \times$$

$$-0.0001 \leq x_4 \leq 0.0001 \quad \times$$

NOTE: $x_0 = 1$ **always**. Its scaling is not changed.

- There are two ways to change the ranges of x :
- Feature scaling
 - Mean normalization

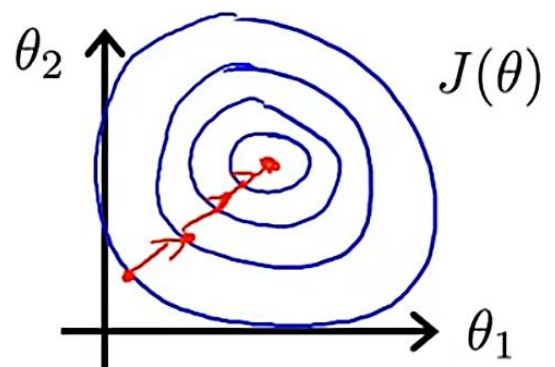
Feature Scaling

Get every feature into approximately a $\boxed{-1 \leq x_i \leq 1}$ range.

$$\rightarrow x_1 = \frac{\text{size (feet}^2\text{)}}{2000} \quad \checkmark$$

$$\rightarrow x_2 = \frac{\text{number of bedrooms}}{5} \quad \checkmark$$

$$0 \leq x_1 \leq 1 \quad 0 \leq x_2 \leq 1$$



- ➔ Feature scaling involves dividing the input values by the range (i.e. the *maximum value minus the minimum value*) of the input variable, resulting in a new range of just 1.
-

Mean normalization

Replace x_i with $x_i - \mu_i$ to make features have approximately zero mean (Do not apply to $x_0 = 1$).

E.g. ➔ $x_1 = \frac{\text{size} - 1000}{2000}$

$x_2 = \frac{\# \text{bedrooms} - 2}{5}$

For x1 : average size = 1000

Range = 2000 = upper limit – lower limit

For x2 : average size = 2

Range = 5

- In mean normalization we try to bring x_i in approx. range:

$$[-0.5 \leq x_1 \leq 0.5] \quad [-0.5 \leq x_2 \leq 0.5]$$

$$x_i := \frac{x_i - \mu_i}{s_i}$$

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

← avg value of x_i in training set
 range (max - min)
 (or standard deviation)

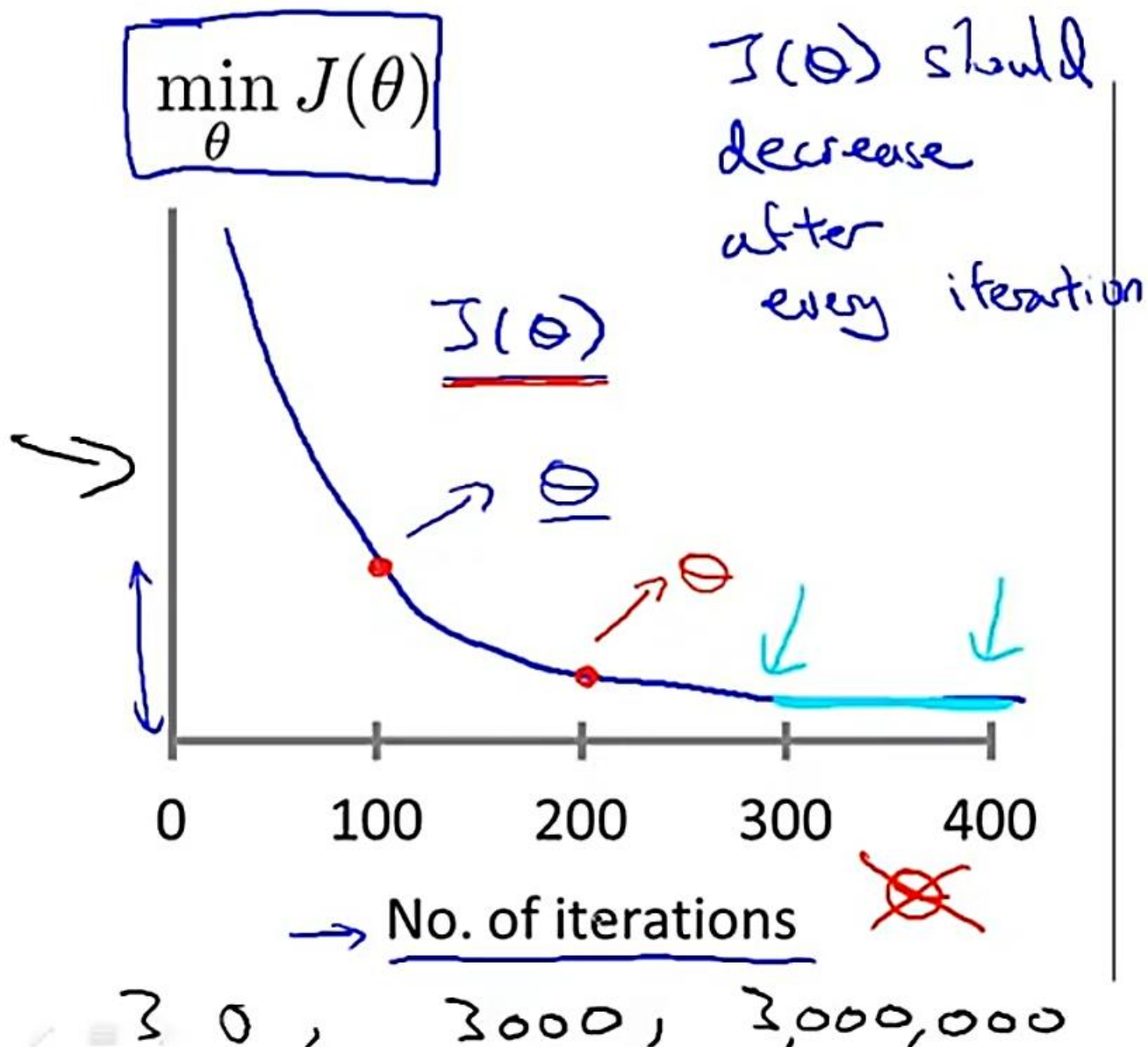
Where μ_i is the **average** of all the values for feature (i) and s_i is the range of values (max - min), or s_i is the standard deviation.

Note that dividing by the range, or dividing by the **standard deviation**, give different results

PRACTICAL TIPS: for grad desc.

- “Debugging”: How to make sure gradient descent is working correctly.
- How to choose learning rate α .

Making sure gradient descent is working correctly:



The goal is to minimize J

Plot **J vs no of iterations**, (not J vs θ): J should decrease after every iteration. In this curve, $J(\theta)$ is the vertical height of that point.

After a time, the **curve flattens** – denoting the convergence has occurred.

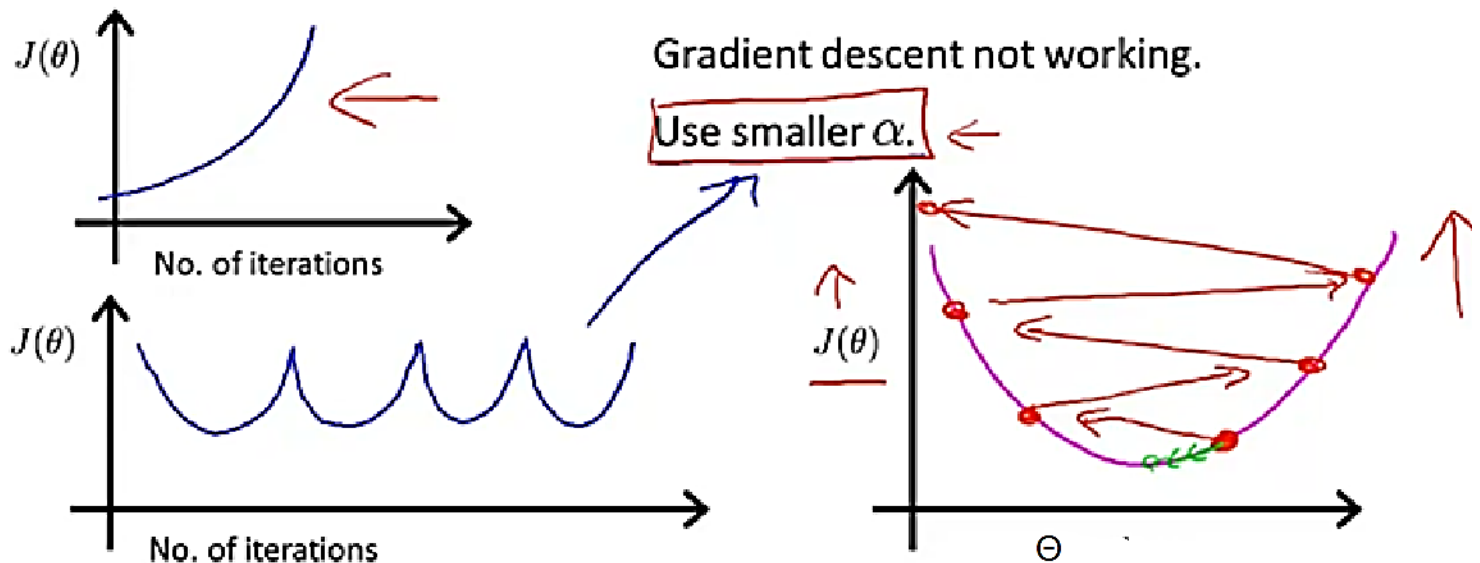
Example automatic convergence test:

Declare convergence if $J(\theta)$ decreases by less than 10^{-3} in one iteration.

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If $J(\theta)$ ever increases, then you probably need to decrease α .

Making sure gradient descent is working correctly.



- For sufficiently small α , $J(\theta)$ should decrease on every iteration. \leftarrow
- But if α is too small, gradient descent can be slow to converge.

All these are **wrong curves** for $J(\theta)$ vs iterations. Solution: use **smaller** values of α .

But not **too small** α as it **slows** the **convergence**. And not too large either: as it may not converge.

To choose α , try

..., 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, ...

\uparrow $\nearrow \times$ $\nearrow \times$ $\nearrow \times$ $\nearrow \times$ $\nearrow \times$ \uparrow \uparrow

$\approx 3\times$ $\approx 3\times$ $\approx 3\times$ $\approx 3\times$

DEFINING NEW FEATURES:

Housing prices prediction

$$h_{\theta}(x) = \theta_0 + \theta_1 \times \underbrace{\text{frontage}}_{x_1} + \theta_2 \times \underbrace{\text{depth}}_{x_2}$$

Area

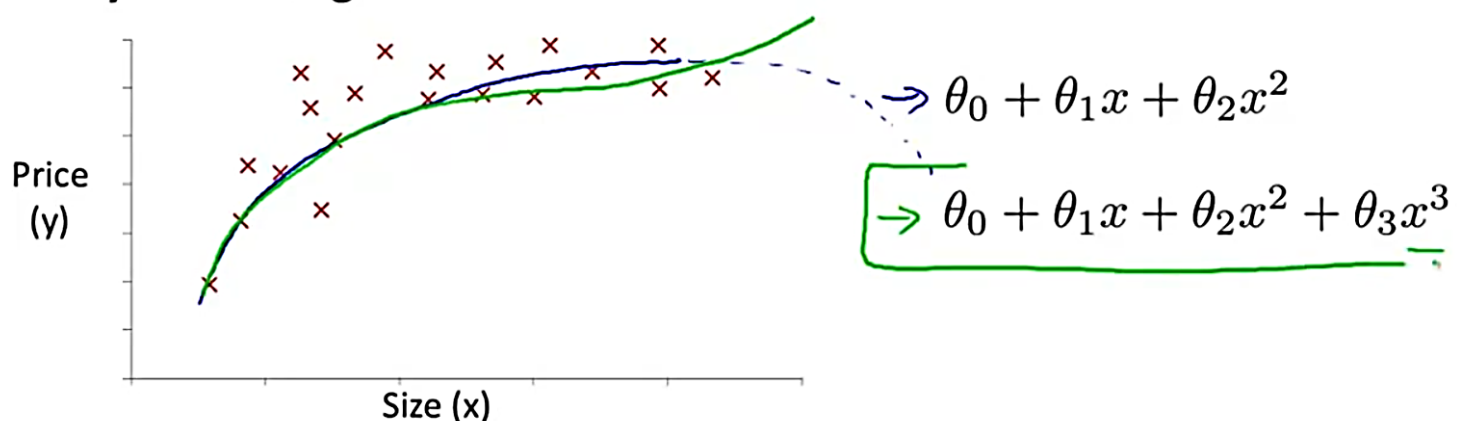
$$x = \underline{\text{frontage} \times \text{depth}}$$

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

↗ land area

POLYNOMIAL REGRESSION: Non-linear hypothesis

Polynomial regression



➔ We can use different hypothesis equations for a single dataset. Whichever best fits logically.

➔ For a multivariate: we can convert all features into functions of each other:

We can **combine** multiple features into one. For example, we can combine x_1 and x_2 into a new feature x_3 by taking $x_1 \cdot x_2$.

Choice of features: We can convert our linear hypothesis into a non-linear one

For example, if our hypothesis function is $h_\theta(x) = \theta_0 + \theta_1 x_1$ then we can create additional features based on x_1 , to get the quadratic function

$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$ or the cubic function $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^3$

Size (x)

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

$$= \theta_0 + \theta_1(\text{size}) + \theta_2(\text{size})^2 + \theta_3(\text{size})^3$$

$\rightarrow x_1 = (\text{size})$
 $\rightarrow x_2 = (\text{size})^2$
 $\rightarrow x_3 = (\text{size})^3$

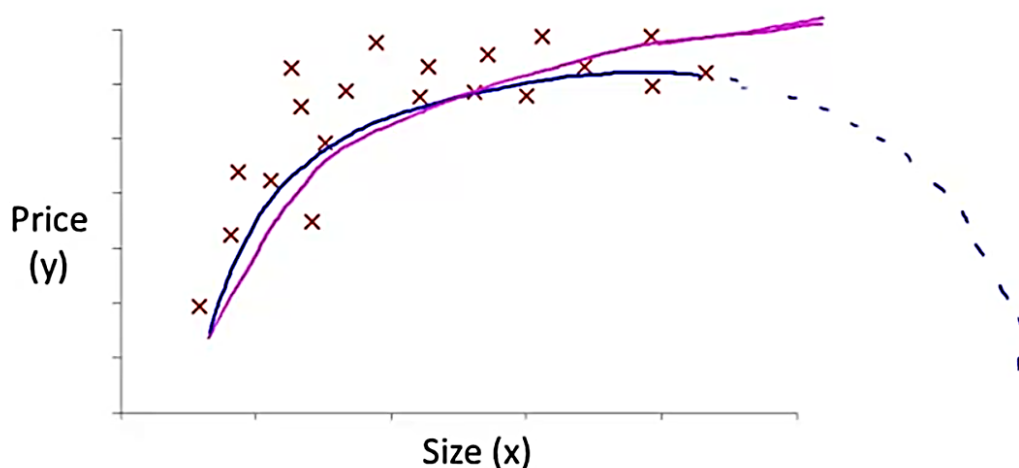
Size: 1 - 1000

Size²: 1 - 1,000,000

Size³: 1 - 10⁹

IMPORTANT: if you choose your features this way then feature scaling becomes very important.

eg. if x_1 has range 1 - 1000 then range of x_1^2 becomes 1 - 1000000 and that of x_1^3 becomes 1 - 1000000000



$\rightarrow h_\theta(x) = \theta_0 + \theta_1(\text{size}) + \theta_2(\text{size})^2$

$\rightarrow h_\theta(x) = \theta_0 + \theta_1(\text{size}) + \theta_2\sqrt{(\text{size})}$



Thus, we find the **best fitting curve** for $h(\Theta)$.

Computing Parameters Analytically:

Up until now, we are using gradient descent Algorithm.. but now we will use new Algo: **NORMAL EQUATIONS**

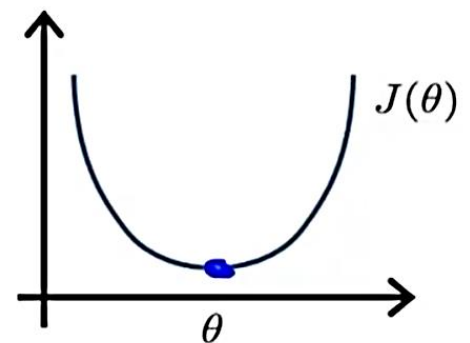
⇒ **NORMAL EQUATIONS**: method to solve for Θ analytically...
unlike grad desc, no need to iterate to minimize the $J(\Theta)$.. its minimized directly in one go.

Intuition: for a **single parameter** Θ :

Intuition: If 1D ($\theta \in \mathbb{R}$)

$$\rightarrow J(\theta) = a\theta^2 + b\theta + c$$
$$\frac{\partial}{\partial \theta} J(\theta) = \dots \stackrel{\text{set}}{=} 0$$

Solve for Θ



For **multiple parameters**:

Θ is a set of m Θ 's.

⇒ For every $\Theta_i \rightarrow$ we set partial derivative of J wrt to $\Theta_i = 0$

- Then we find Θ corresponding to that eqn
- This is done for each Θ

$$\theta \in \mathbb{R}^{n+1} \quad J(\theta_0, \theta_1, \dots, \theta_m) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$
$$\frac{\partial}{\partial \theta_j} J(\theta) = \dots \stackrel{\text{set}}{=} 0 \quad (\text{for every } j)$$

Solve for $\theta_0, \theta_1, \dots, \theta_n$

Examples: $m = 4$.

	Size (feet ²)	Number of bedrooms	Number of floors	Age of home (years)	Price (\$1000)
x_0	x_1	x_2	x_3	x_4	y
1	2104	5	1	45	460
1	1416	3	2	40	232
1	1534	3	2	30	315
1	852	2	1	36	178

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix}$$

$m \times (n+1)$

$$y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$

m -dimensional vector

m = number of example datas

n = no of features in input

$n + 1 \Rightarrow$ we give an extra feature $x_0=1$ to every example.

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

\Rightarrow To construct the X matrix from x_i vectors:

- **Transpose** them and fill into the X matrix, Such that the x 's belonging to a single example.. comes in row

m examples $(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})$; n features.

$$\underline{x^{(i)}} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix} \in \mathbb{R}^{n+1} \quad \bigg| \quad X = \begin{bmatrix} \text{---} (x^{(1)})^T \text{---} \\ \text{---} (x^{(2)})^T \text{---} \\ \vdots \\ \text{---} (x^{(m)})^T \text{---} \end{bmatrix}$$

(design matrix)

E.g. If $\underline{x}^{(i)} = \begin{bmatrix} 1 \\ x_1^{(i)} \end{bmatrix}$ \rightarrow $\underline{X} = \begin{bmatrix} 1 & x_1^{(1)} \\ \vdots & \vdots \\ 1 & x_1^{(m)} \end{bmatrix}$ \cdot $\underline{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}$

$m \times (n+1)$ $m \times 2$

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In above example : for all m training sets there are only 2 features x_0 and x_1 .

Octave: $\text{pinv}(\underline{X}' * \underline{X}) * \underline{X}' * \underline{y}$

$\text{pinv}(\underline{X}^T * \underline{X}) * \underline{X}^T * \underline{y}$

$\underline{\theta} = (\underline{X}^T \underline{X})^{-1} \underline{X}^T \underline{y}$ $\min_{\underline{\theta}} J(\underline{\theta})$

\underline{X}' \underline{X}^T

~~Feature Scaling~~

$0 \leq x_1 \leq 1$
 $0 \leq x_2 \leq 1000$
 $0 \leq x_3 \leq 10^{-5}$ ✓

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\underline{X}' = transpose of \underline{X}

\Rightarrow **Feature scaling is not required in Normal Equations**
 method(algo)..Unlike in gradient desc \Rightarrow in which its req

WHEN TO USE GRAD DESC v/s NORMAL EQN:

m training examples, n features.

Gradient Descent

- \rightarrow • Need to choose α .
- \rightarrow • Needs many iterations.
- Works well even when n is large.

$\underline{n} = 10^6$

\underline{X} is $m \times (n+1)$

Normal Equation

- \rightarrow • No need to choose α .
- \rightarrow • Don't need to iterate.
- Need to compute $(\underline{X}^T \underline{X})^{-1}$ $(n+1) \times (n+1)$ $O(n^3)$
- Slow if n is very large.

$n = 100$
 $n = 1000$
 $n = 10000$

$O(kn^2)$

$O(n^3)$, need to calculate inverse of $\underline{X}^T \underline{X}$

When **no. of features is small** (upto 10^5) => use **normal eqns.**

As for **large value of n** => $X' * X$ will be a $n \times n$ matrix: and we have to find its inverse:

Inverse is of complexity $O(n^3)$ => thus for **large no. of input features**, **grad desc** is better way to converge to minima.

NON INVERTIBILITY PROBLEM IN NORMAL EQN METHOD:

Sometimes $X' * X$ is not invertible (singular/degenerate)..:

REASONS:

Redundant features – two columns or rows are proportional in the $X' * X$ matrix. (i.e. they are linearly dependent)

⇒ **SOLUTION:** delete one of the dependent features.

Too many features – the number of features is too large as compares to no of examples... ($m \ll n$)

⇒ **SOLUTION:** delete some features or Use **REGULARIZATION TECHNIQUE.**

\$OCTAVE: $\text{pinv}(X' * X) * X' * y$

⇒ this would still give the right value of Θ . (Even if $X' * X$ is non invertible).

⇒ $\text{pinv}()$ is pseudo inverse

⇒ $\text{inv}()$ is just inverse
