Overview

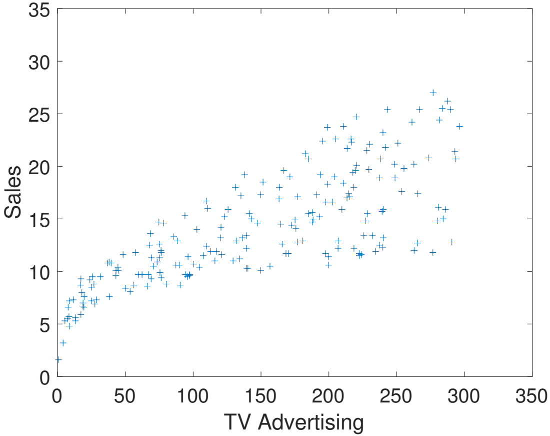
- Linear Regression with One Variable
- Gradient Descent
- Linear Regression with Multiple Variables
- Gradient Descent with Multiple Variables

Example: Advertising Data

- Data taken from An Introduction to Statistical Learning with Applications in R (http://www-bcf.usc.edu/~gareth/ISL/data.html)
- Data consists of the advertising budgets for three media (TV, radio and newspapers) and the overall sales in 200 different markets.

TV	Radio	Newspaper	Sales
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	9.3
⋮	⋮	⋮	⋮

Example: Advertising Data



- Suppose we want to predict sales in a new area ?
- Predict sales when the TV advertising budget is increased to 350 ?
- ... Draw a line that fits through the data points

Some Notation

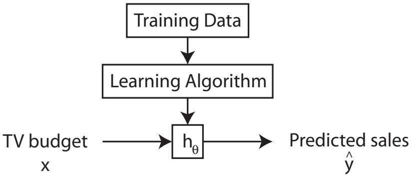
Training data:

TV (x)	Sales (y)
230.1	22.1
44.5	10.4
17.2	9.3
$\vdots$	$\vdots$

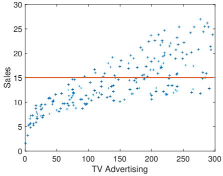
- m=number of training examples
- x="input" variable/features
- y="output" variable/"target" variable

- $(x^{(i)}, y^{(i)})$ the ith training example
- $x^{(1)} = 230.1$, $y^{(1)} = 22.1$, $x^{(2)} = 44.5$, $y^{(2)} = 10.4$

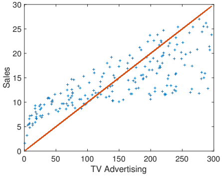
Model Representation



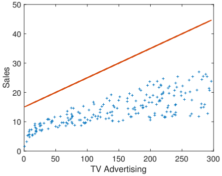
- Prediction:
  $\hat{y} = h_\theta(x) = \theta_0 + \theta_1 x$
- θ_0, θ_1 are (unknown) parameters
- sometimes abbreviate $h_\theta(x)$ to $h(x)$



$\theta_0 = 15,\ \theta_1 = 0$



$\theta_0 = 0,\ \theta_1 = 0.1$

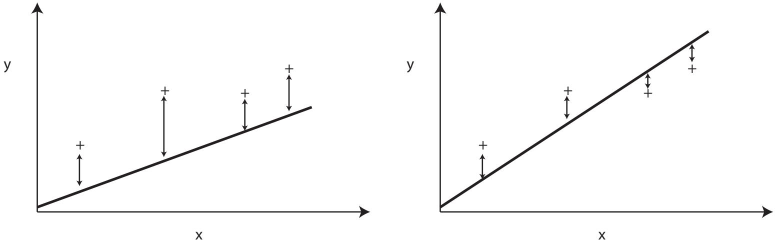


$\theta_0 = 15,\ \theta_1 = 0.1$

Cost Function: How to choose model parameters θ?

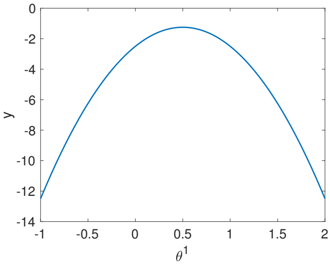
- Prediction: $\hat{y} = h_\theta(x) = \theta_0 + \theta_1 x$
- Idea: Choose θ_0 and θ_1 so that $h_\theta(x^{(i)})$ is close to $y^{(i)}$ for each of our training examples $(x^{(i)}, y^{(i)})$, $i = 1, \dots, m$.
- Least squares case: select the values for θ_0 and θ_1 that minimise cost function:

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

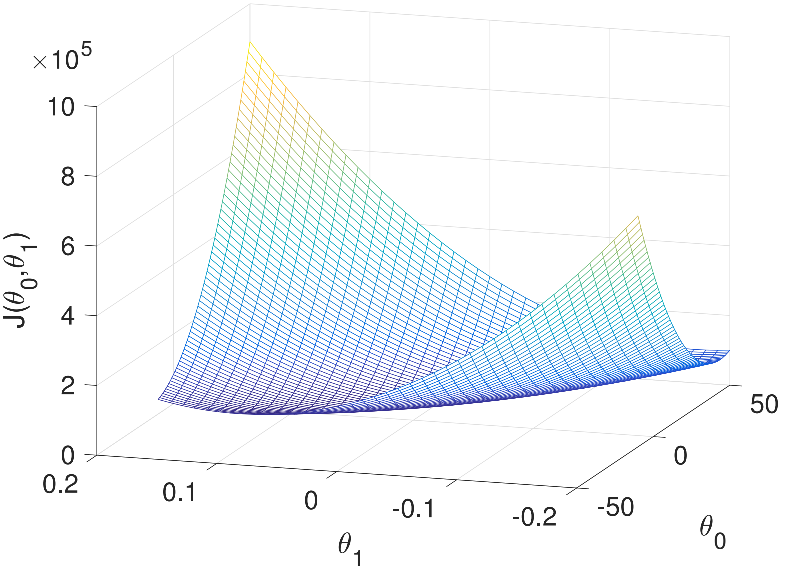


Simple Example

- Suppose our training data consists of just two observations: $(3,1)$, $(2,1)$, and to keep things simple we know that $\theta_0 = 0$.
- The cost function is $\frac{1}{2}\sum_{j=1}^{2}(y^{(j)} + \theta_1 x^{(j)})^2 = \frac{1}{2}(1-3\theta_1)^2 + (2-1\theta_1)^2$
- What value of θ_1 minimises $(1-3\theta_1)^2 + (2-1\theta_1)^2$?

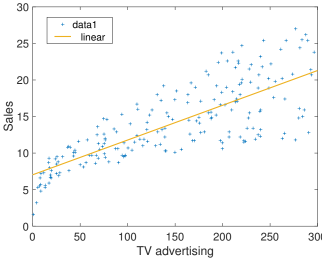


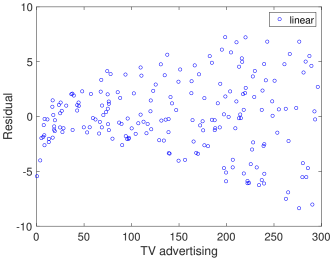
Example: Advertising Data



Example: Advertising Data

- Least square linear fit
- Residuals are the difference between the value predicted by the fit and the measured value.
  - Do the residuals look "random" or do they have some "structure" ? Is our model satisfactory ?
  - We can use the residuals to estimate a confidence interval for the prediction made by our linear fit.
- We could use cross-validation/bootstrapping to estimate out confidence in the fit itself.





Summary

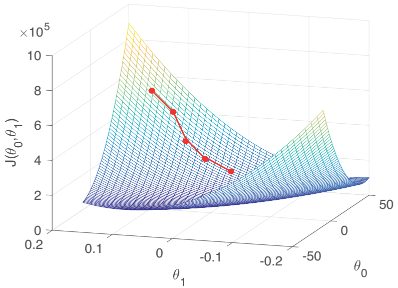
- Hypothesis: $h_\theta(x) = \theta_0 + \theta_1 x$
- Parameters: θ_0, θ_1
- Cost Function: $J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$
- Goal: Select θ_0 and θ_1 that minimise $J(\theta_0, \theta_1)$

Gradient Descent

Need to select θ_0 and θ_1 that minimise $J(\theta_0, \theta_1)$. Brute force search over pairs of values of θ_0 and θ_1 is inefficient, can we be smarter ?

- Start with some θ_0 and θ_1
- Repeat:

  Update θ_0 and θ_1 to new value which makes $J(\theta_0, \theta_1)$ smaller

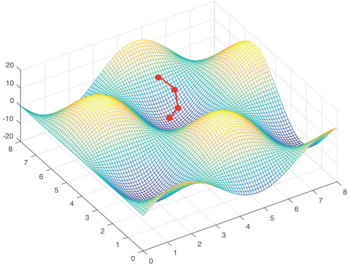


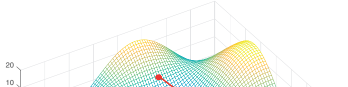
- When curve is "bowl shaped" or convex then this must eventually find the minimum.

Gradient Descent

- Start with some θ_0 and θ_1
- Repeat:

  Update θ_0 and θ_1 to new value which makes $J(\theta_0, \theta_1)$ smaller
- When curve has several minima then we can't be sure which we will converge to.
- Might converge to a local minimum, not the global minimum



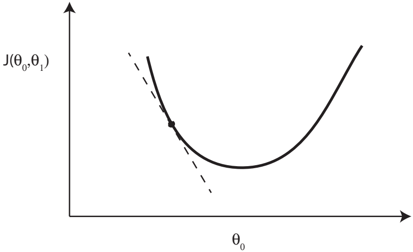


Gradient Descent

Repeat: Update θ_0 and θ_1 to new value which makes $J(\theta_0, \theta_1)$ smaller

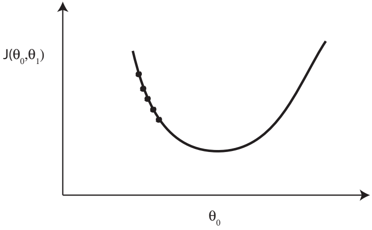
- One option: carry out local search of θ_0 and θ_1 to find one that decreases J.
- Another option: gradient descent:

$$\begin{aligned} temp0 &:= \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \\ temp1 &:= \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) \\ \theta_0 := temp0,&\ \theta_1 := temp1 \end{aligned}$$



- $\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \approx \frac{J(\theta_0+\delta, \theta_1) - J(\theta_0, \theta_1)}{\delta}$ for δ sufficiently small.
- $J(\theta_0 + \delta, \theta_1) \approx J(\theta_0, \theta_1) + \delta \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$
- When $\delta = -\alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$ then $J(\theta_0 + \delta, \theta_1) \approx J(\theta_0, \theta_1) - \alpha \left(\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \right)^2$

Gradient Descent



- Selecting step size α too small will mean it takes a long time to converge to minimum
- But selecting α too large can lead to us overshooting the minimum
- We need to adjust α so that algorithm converges in a reasonable time.

Gradient Descent

For $J(\theta_0, \theta_1) = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$ with $h_\theta(x) = \theta_0 + \theta_1 x$:

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

So gradient descent algorithm is:

- repeat:

$$
\begin{aligned}
&temp0 := \theta_0 - \frac{2\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})\\
&temp1 := \theta_1 - \frac{2\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x^{(i)}\\
&\theta_0 := temp0,\ \ \theta_1 := temp1
\end{aligned}
$$

Linear Algebra Review

Its assumed you know basic linear algebra for this module. There is lots of revision material online e.g.

- https://youtu.be/6AP4IvfKmwg (coursera linear algebra review)
- https://www.khanacademy.org/math/linear-algebra

Basic notation:

- Vector $x = \left[\begin{array}{c} 230.1 \\ 37.8 \end{array} \right]$, element $x_1 = 230.1$
- Matrix $A = \left[\begin{array}{cc} 1 & 2 \\ 3 & 4 \end{array} \right]$, element $A_{11} = 1$
- Transpose $x^T = [230.1\ 37.8]$
- Inner product $x^T y = \sum_{i=1}^{n} x_i y_i$ for two vectors with n elements
- Produt of a matrix and a vector Ax, product of two matrices AB.

Linear Regression with Multiple Variables

Advertising example:

TV x_1	Radio x_2	Newspaper x_3	Sales y
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	9.3
$\vdots$	$\vdots$	$\vdots$	$\vdots$

- n=number of features (3 in this example)
- $(x^{(i)}, y^{(i)})$ the ith training example e.g.
  $$x^{(1)} = [230.1, 37.8, 69.2]^T = \begin{bmatrix} 230.1 \\ 37.8 \\ 69.2 \end{bmatrix}$$
- $x_j^{(i)}$ is feature j in the ith training example, e.g. $x_2^{(1)} = 37.8$

Linear Regression with Multiple Variables

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

e.g. $\underbrace{h_\theta(x)}_{Sales} = 15 + 0.1 \underbrace{x_1}_{TV} - 5 \underbrace{x_2}_{Radio} + 10 \underbrace{x_3}_{Newspaper}$

- For convenience, define $x_0 = 1$
  i.e. $x_0^{(1)} = 1$, $x_0^{(2)} = 1$ etc
- Feature vector $x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$
- Parameter vector $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$
- $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n = \theta^T x$

Linear Regression with Multiple Variables

- Hypothesis: $h_\theta(x) = \theta^T x$ (with θ, x now $n+1$-dimensional vectors)
- Cost Function: $J(\theta_0, \theta_1, \ldots, \theta_n) = J(\theta) = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$
- Goal: Select θ that minimises $J(\theta)$

As before, can find θ using:

- Start with some θ
- Repeat:

  Update vector θ to new value which makes $J(\theta)$ smaller

e.g using gradient descent:

- Start with some θ
- Repeat:

  for j=0 to n $\{tempj := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)\}$

  for j=0 to n $\{\theta_j := tempj\}$

Gradient Descent with Multiple Variables

For $J(\theta) = \sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$ with $h_\theta(x) = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$:

- $\frac{\partial}{\partial\theta_0} J(\theta) = \frac{2}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})$
- $\frac{\partial}{\partial\theta_1} J(\theta) = \frac{2}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_1^{(i)}$
- $\frac{\partial}{\partial\theta_j} J(\theta) = \frac{2}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$

So gradient descent algorithm is:

- Start with some θ
- Repeat:

  for j=0 to n $\{tempj := \theta_j - \frac{2\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}\}$
  for j=0 to n $\{\theta_j := tempj\}$

Example: Advertising Data

- How is the impact of the advertising spend on TV and radio related, if at all ?
- Perhaps a quadratic fit would be better ? If so, what does that imply for how we allocate our advertising budget ?