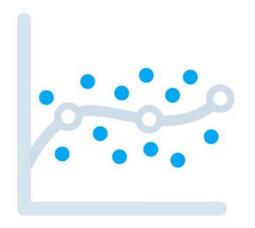
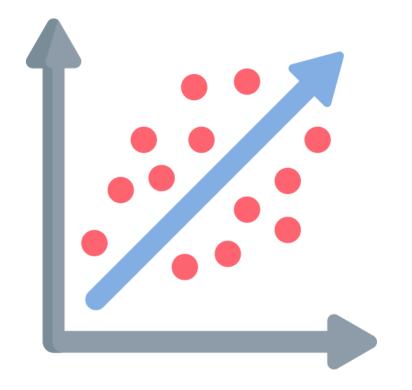
Regression



Outline

- Linear Regression with One Variable
- Multiple Linear Regression
- Polynomial Regression
- Regression Practical Considerations

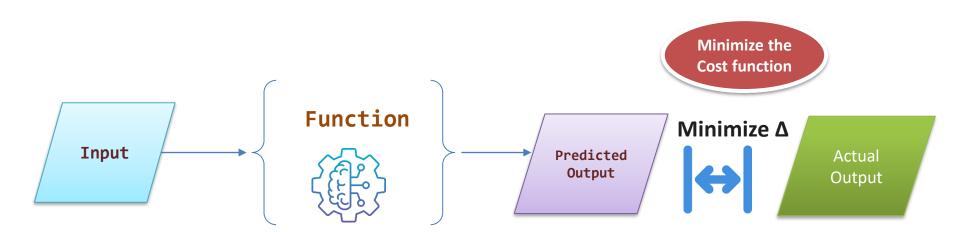
Linear Regression with One Variable





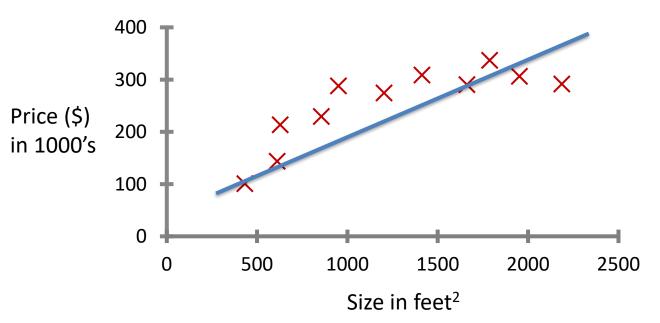
ML: learn a Function that minimizes the cost

- Start with random function parameters
- Repeat intelligent guessing/approximation of the Function parameters such that the difference between the Predicted Output the Actual Output is reduced
 - i.e., minimize a Cost function a.k.a loss, or error function



Linear Regression with One Variable





regression with one variable aka Univariate linear regression

- <u>Regression</u>: Predict continuous output value (e.g., price)
- Linear regression is used to predict the value of a variable based on the value of another variable(s)
- Linear regression fits a straight line that minimizes the discrepancies between predicted and actual output values

Training	set of
housing	prices

Size in feet ² (x)	Price (\$) in 1000's (<i>y</i>)
2104	460
1416	232
1534	315
852	178
•••	•••

Notation:

m = Number of training examples

$$(x^{(i)}, y^{(i)})$$
 – the *i*th training example

$$x^{(1)} = 2104$$

$$x^{(2)} = 1416$$

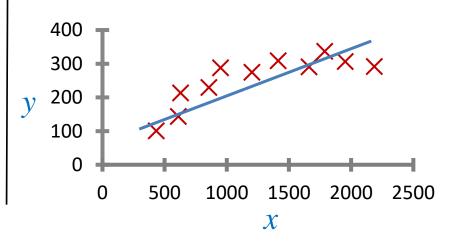
$$y^{(1)} = 460$$

Training Set Learning Algorithm Y hat Size of **Estimated** house price

How do we represent f?

$$f(x) = wx + b$$

w, b are parameters (coefficients)to learn from the training set



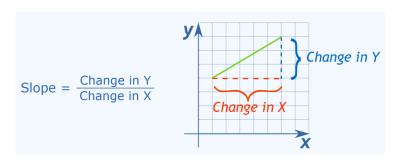
- Given a training set, **learn a function** f so that f(x) is a "good" predictor for the corresponding value of y
- Find w, b parameters that minimize the error between predicted and actual values (i.e., minimize $\frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i-y_i)^2$ for all dataset instances)

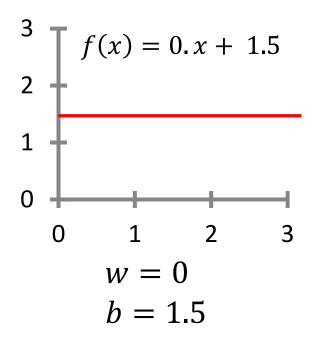
Univariate Linear Regression - Model Representation

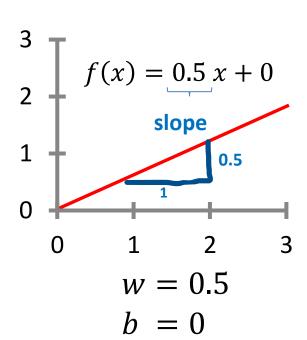
$$f(x) = wx + b$$

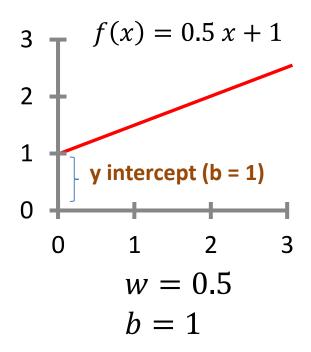
- w is the slope of the line
- b is the y-intercept of the line

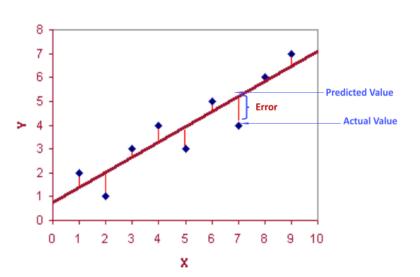
How to choose w and b?











Idea: Find w and b so that f(x) is close to y for our training examples (x, y)

Find w, b: $\hat{y}^{(i)}$ is close to $y^{(i)}$ for all $(x^{(i)}, y^{(i)})$

Cost (mean squared error)

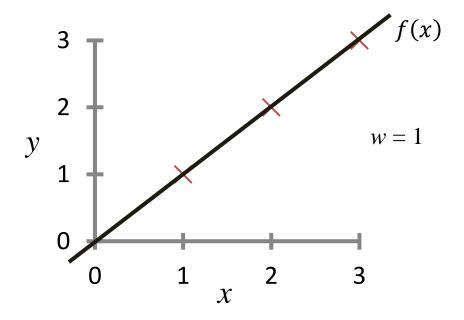
Function:

$$J(w,b) = \frac{1}{2m} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2 = \frac{1}{2m} \sum_{i=1}^{m} (f(x^{(i)}) - y^{(i)})^2$$

Goal: minimize J(w, b)

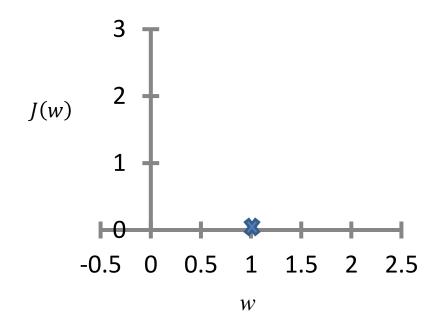
With m = number of training examples

$$f(x) = wx$$



$$J(w) = \frac{1}{2m} \sum_{i=1}^{m} (f(x^{(i)}) - y^{(i)})^2$$
$$= \frac{1}{2m} (0^2 + 0^2 + 0^2) = 0$$

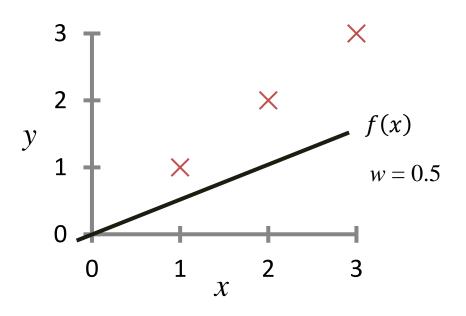
For simplicity, let us assume our optimization objective is to $\underset{w,b}{\text{minimize}} J(w)$, thus, b = 0





slides\regression.xlsx

$$f(x) = wx$$

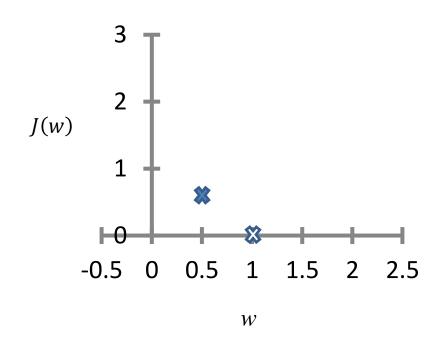


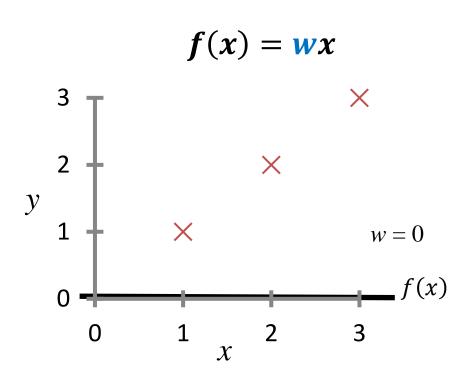
$$J(w) = \frac{1}{2m} \sum_{i=1}^{m} (f(x^{(i)}) - y^{(i)})^2$$

$$= \frac{1}{2m} ((0.5 - 1)^2 + (1-2)^2 + (1.5-3)^2)$$

$$= \frac{1}{2 \times 3} (3.5) = \frac{3.5}{6} = 0.58$$

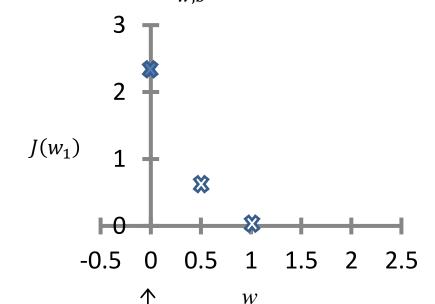
For simplicity, let us assume our optimization objective is to minimize J(w), thus, b = 0

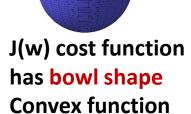


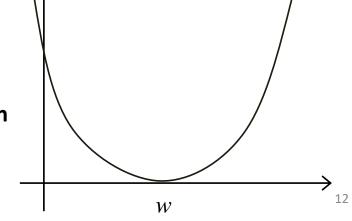


$$J(w) = \frac{1}{2m} \sum_{i=1}^{m} (f(x^{(i)}) - y^{(i)})^{2}$$
$$= \frac{1}{2m} (1^{2} + 2^{2} + 3^{2})$$
$$= \frac{1}{2 \times 3} (14) = \frac{14}{6} = 2.3$$

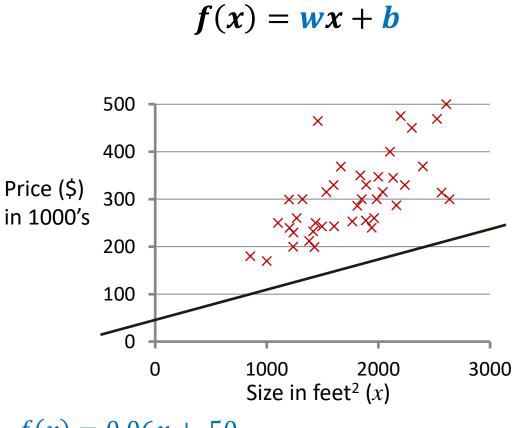
For simplicity, let us assume our optimization objective is to minimize J(w), thus, b = 0

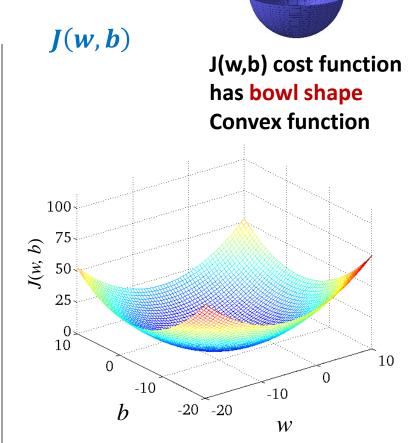






J(w)



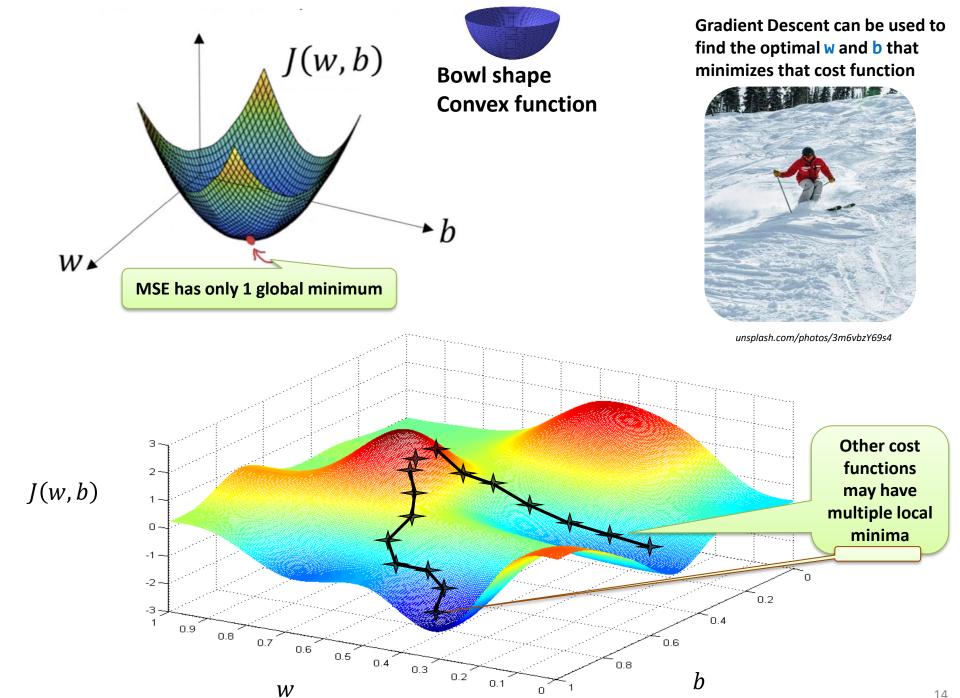


$$f(x) = 0.06x + 50$$

- The fact that the cost function squares the error ensures that the 'error surface' is **convex** like a soup bowl.
- It will always have a minimum that can be reached by following the **gradient** (i.e., the slope)
- Minimizing the cost function yields optimal values of w and b



08.regression\02_cost_function.py



Gradient descent algorithm

Want to find w and b that minimize the cost function J

$$\underset{w,b}{\operatorname{minimize}} \boldsymbol{J}(\boldsymbol{w},\boldsymbol{b})$$

- 1. Initialize the values of \mathbf{w} and \mathbf{b} to some arbitrary values (say 0, 0)
- 2. Calculate the predicted values of \mathbf{y} using the current values of \mathbf{w} and \mathbf{b}
- 3. Calculate the gradients of the cost function with respect to \mathbf{w} and \boldsymbol{b}
- 4. Update the values of **w** and **b** using the gradients and a learning rate

Learning Rate

$$\omega = \omega - \omega \frac{\partial}{\partial w} J(w,b)$$

Derivative of the Cost Function w.r.t w

 $\omega = b - \alpha \frac{\partial}{\partial b} J(w,b)$

5. Repeat steps 2-4 until convergence (i.e., until the cost function converges to a minimum)

Gradient descent algorithm

Gradient descent utilizes the partial derivative of the cost function with respect to \mathbf{w} and \mathbf{b} to update \mathbf{w} and \mathbf{b} parameters

Repeat until convergence {

$$w = w - \alpha \frac{1}{m} \sum_{i=1}^{m} (\hat{\mathbf{y}}^{(i)} - y^{(i)}) \cdot x^{(i)}$$

$$\frac{\partial}{\partial w} J(w)$$

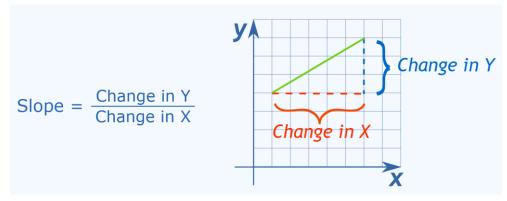
$$b = b - \alpha \frac{1}{m} \sum_{i=1}^{m} (\hat{\mathbf{y}}^{(i)} - \mathbf{y}^{(i)})$$

$$\frac{\partial}{\partial b} J(b)$$

(simultaneously update w and b)

Derivative 101

- Source https://www.mathsisfun.com/calculus/derivatives-introduction.html
- **Derivatives**: it is all about slope!



We can find an **average** slope between two points

average slope =
$$\frac{24}{15}$$

Derivative = slope at a point

- Fill in this slope formula: $\frac{\Delta y}{\Delta x} = \frac{f(x+\Delta x) f(x)}{\Delta x}$
- Simplify it as best we can
- Then make Δx shrink towards zero.

Example

The slope formula is:
$$\frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Use
$$f(x) = x^2$$
:
$$\frac{(x+\Delta x)^2 - x^2}{\Delta x}$$

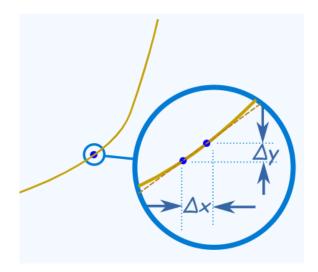
Expand
$$(x+\Delta x)^2$$
 to x^2+2x $\Delta x+(\Delta x)^2$: $\frac{x^2+2x$ $\Delta x+(\Delta x)^2-x^2}{\Delta x}$

Simplify (x² and -x² cancel):
$$\frac{2x \Delta x + (\Delta x)^2}{\Delta x}$$

Simplify more (divide through by Δx): $2x + \Delta x$

Then, as Δx heads towards 0 we get: 2x

Result: the derivative of x^2 is 2x



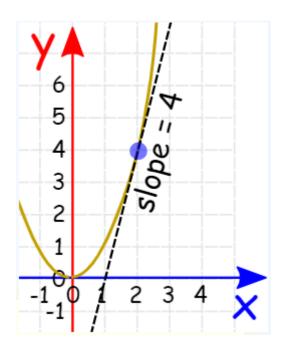
$$\frac{d}{dx}x^2 = 2x$$

In other words, the slope at x is 2x

Interpretation of Derivative

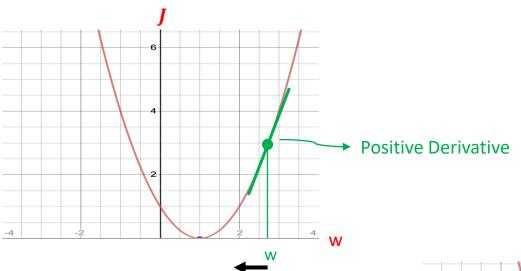
- So what does $\frac{d}{dx}x^2 = 2x$ mean?

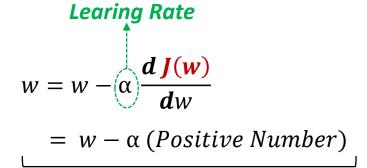
- It means that, for the function x², the slope or "rate of change" at any point is **2**x
- So, when x=2 the slope is 2x = 4
- Or when x=5 the slope is 2x = 10, and so on



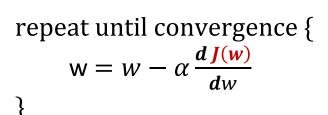
The Impact of Partial Derviative

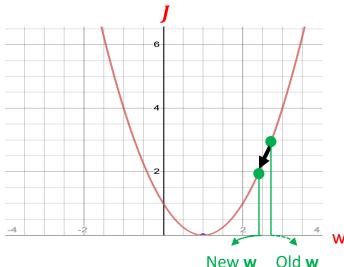
• For simplicity, let us assume our optimization objective is to minimize J(w), thus, b = 0





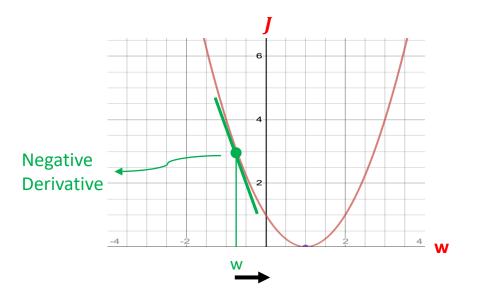
Decrease \boldsymbol{w} by a certain value





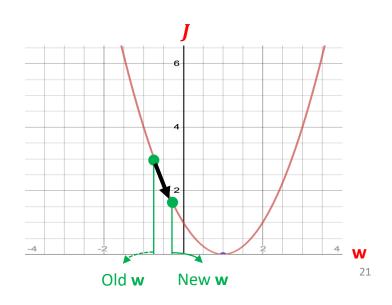
The Impact of Partial Derviative

• For simplicity, let us assume our optimization objective is to minimize J(w), thus, b = 0 w,b



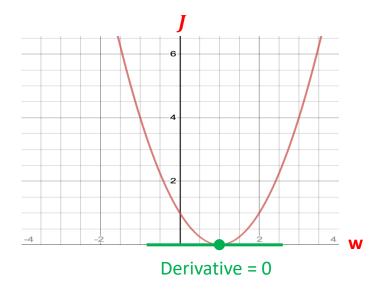
$$w = w - \alpha \frac{dJ(w)}{dw}$$
$$= w - \alpha (Negative Number)$$

Increase \boldsymbol{w} by a certain value



The Impact of Partial Derviative

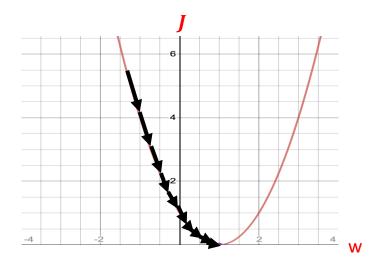
• For simplicity, let us assume our optimization objective is to minimize J(w), thus, b = 0

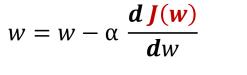


$$w = w - \alpha \frac{dJ(w)}{dw}$$
$$= w - \alpha (Zero)$$

w remains the same, hence, gradient descent converges

The Impact of Learning Rate

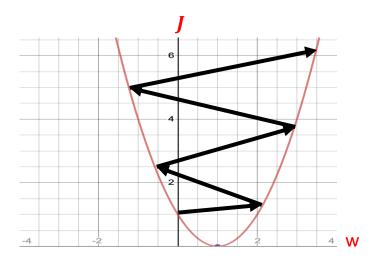




What happens if α is too small?

$$= w - (Too Small Number) \frac{d J(w)}{dw}$$

w changes only a tiny bit on each step, hence, gradient descent will render slow (will take more time to converge)



$$w = w - \alpha \frac{dJ(w)}{dw}$$

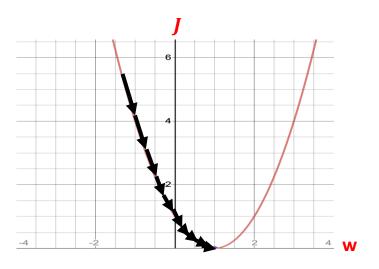
What happens if α is too large?

$$= w - (Too\ Large\ Number)\ \frac{d\ J(w)}{dw}$$

w changes a lot (and probably faster) on each step, hence, gradient descent will potentially overshoot the minimum and, accordingly, fail to converge (or even diverge)

The Impact of Learning Rate

We can set α between 0 and 1 (say, 0.1, or a little more or less, hence, not very small or very large)



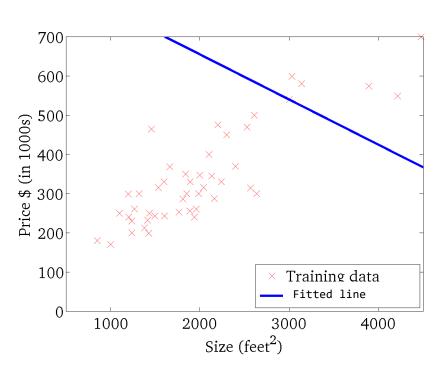
$$w = w - \alpha \, \frac{d J(w)}{dw}$$

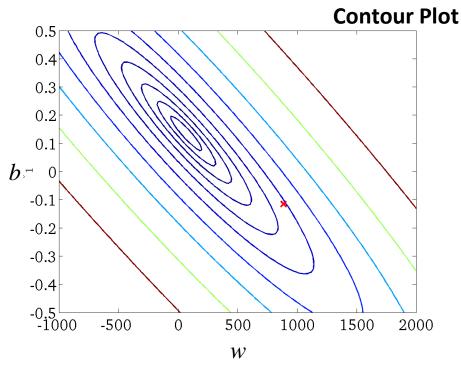
α remains fix. As we approach the minimum, gradient descent will automatically start taking smaller steps (i.e., w will start changing at a slower pace because the derivative will become less steep)

Visualizing gradient descent algorithm

$$f(x) = wx + b$$

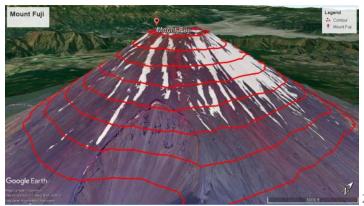
J(w,b)



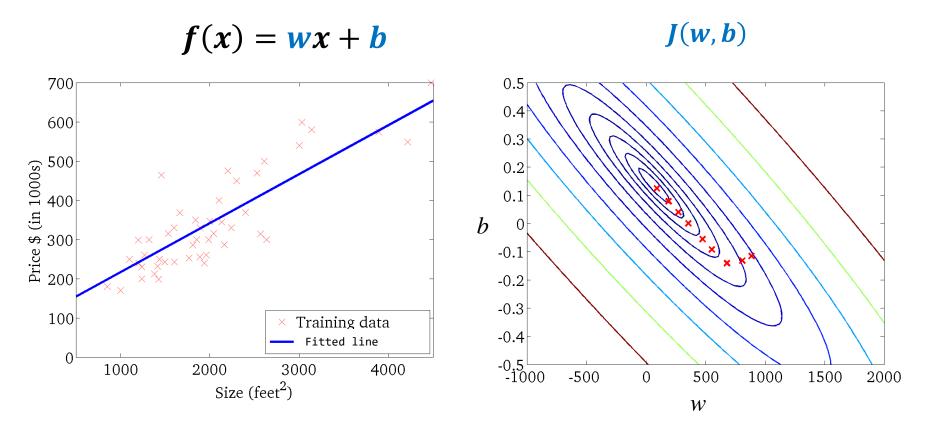


The optimal values of w and b are in the center of the inner most 'circle' of the Contour Plot





Visualizing gradient descent algorithm

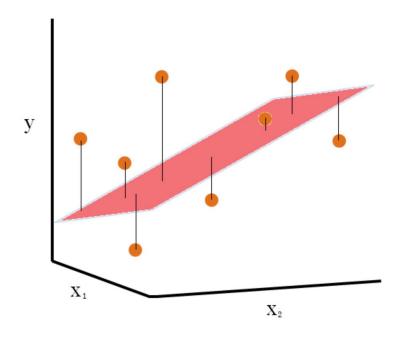


- The contour plot shows J(w, b) over a range of w and b. The cost levels are represented by the rings
- The red crosses is the **path of gradient descent**. The path makes steady progress toward its goal. The initial steps are much larger than the steps near the goal.
- The optimal values of w and b are in the center of the inner most 'circle' of the Contour Plot

Different modes of gradient descent

- Batch Gradient Descent (BGD): Each iteration of gradient descent uses all the training examples
 - It provides a precise estimate of the gradient but can be computationally expensive, especially for large datasets
- Stochastic Gradient Descent (SGD): only a random sample from the dataset is used to compute the gradient in each iteration
 - It is computationally more efficient
 - However, it introduces more noise in the parameter updates, leading to more oscillations in the convergence path
- Mini-Batch Gradient Descent: divides the dataset into small mini-batches and computes the gradient using a mini-batch in each iteration
 - This approach combines the efficiency of stochastic gradient descent with the stability of batch gradient descent

Multiple Linear Regression





Linear Regression with multiple variables

Multiple features (variables)

Size (feet²)	Number of bedrooms	Number of floors	Age of home (years)	Price (\$1000)
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
•••	•••	•••		•••

Notation:

n = number of features $\mathbf{x}_{j} = \mathbf{j}^{th}$ feature $\mathbf{x}^{(i)}$ = features of i^{th} training example $x_{j}^{(i)}$ = value of feature j in i^{th} training example

Multiple Linear Regression - Model Representation

Univariate Linear Regression: f(x) = wx + b

Multiple Linear Regression:

$$f(x) = w_1 x_1 + w_2 x_2 + \dots + w_n x_n + b$$

Example $f(x) = 0.1 \chi_1 + 4 \chi_2 + 10 \chi_3 + -2 \chi_4 + 80$ size #bedrooms #floors years price

$$f_{W,b}(\vec{x}) = w_1 x_1 + w_2 x_2 + \dots + w_n x_n + b$$

$$\vec{w} = [w_1 \ w_2 \ w_3 \dots w_n] \quad \text{parameters} \quad \text{of the model}$$

$$b \text{ is a number}$$

$$vector \vec{\chi} = [\chi_1 \ \chi_2 \ \chi_3 \dots \chi_n]$$

$$f_{\overrightarrow{W},b}(\overrightarrow{x}) = \overrightarrow{w} \cdot \overrightarrow{x} + b = w_1 X_1 + w_2 X_2 + w_3 X_3 + \cdots + w_n X_n + b$$

$$dot product$$

Multiple Linear Regression - Model Representation

Parameters and features

$$\overrightarrow{w} = \begin{bmatrix} w_1 & w_2 & w_3 \end{bmatrix}$$
 $n = 3$
b is a number $\overrightarrow{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}$

linear algebra: count from 1



code: count from 0

Without vectorization

$$f_{\overrightarrow{w},b}(\overrightarrow{x}) = w_1 x_1 + w_2 x_2 + w_3 x_3 + b$$

$$f = w[0] * x[0] + w[1] * x[1] + w[2] * x[2] + b$$



Without vectorization

$$f_{\overrightarrow{\mathbf{w}},b}(\overrightarrow{\mathbf{x}}) = \left(\sum_{j=1}^{n} w_j x_j\right) + b$$



Vectorization

$$f_{\overrightarrow{\mathbf{w}},b}(\overrightarrow{\mathbf{x}}) = \overrightarrow{\mathbf{w}} \cdot \overrightarrow{\mathbf{x}} + b$$

$$f = np.dot(w, x) + b$$



Previous notation

Vector notation

Model

$$w_1, \cdots, w_n$$
 b

$$f_{\overrightarrow{\mathbf{W}},b}(\overrightarrow{\mathbf{X}}) = w_1 x_1 + \dots + w_n x_n + b$$

Cost function
$$J(w_1, \dots, w_n, b)$$

$$J(w_1, \cdots, w_n, b)$$

Gradient descent

repeat {
$$w_j = w_j - \alpha \frac{\partial}{\partial w_j} J(w_1, \dots, w_n, b)$$

$$b = b - \alpha \frac{\partial}{\partial b} J(w_1, \dots, w_n, b)$$
 }

$$\overrightarrow{\mathbf{w}} = \begin{bmatrix} w_1 & \cdots & w_n \end{bmatrix}$$

$$b$$

$$f_{\overrightarrow{\mathbf{w}},b}(\overrightarrow{\mathbf{x}}) = \overrightarrow{\mathbf{w}} \cdot \overrightarrow{\mathbf{x}} + b$$

$$\mathbf{w} \cdot \overrightarrow{\mathbf{x}} + b$$

repeat {
$$w_{j} = w_{j} - \alpha \frac{\partial}{\partial w_{j}} J(\overrightarrow{w}, b)$$

$$b = b - \alpha \frac{\partial}{\partial b} J(\overrightarrow{w}) b$$
}

Gradient Descent

One feature

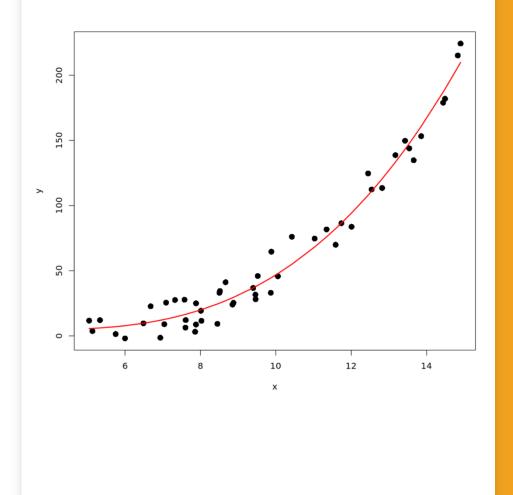
repeat {

$$\underline{w} = w - \alpha \frac{1}{m} \sum_{i=1}^{m} (f_{w,b}(x^{(i)}) - y^{(i)}) x^{(i)}$$
$$\frac{\partial}{\partial w} J(w,b)$$

$$b = b - \alpha \frac{1}{m} \sum_{i=1}^{m} (f_{w,b}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)})$$

n features $(n \ge 2)$

Polynomial Regression

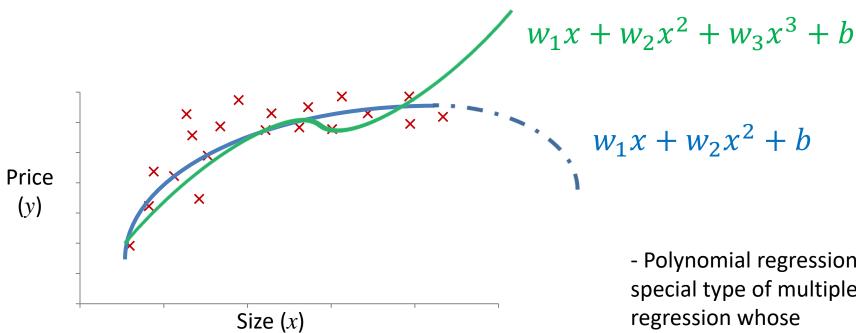




Polynomial Regression

- When the relationship between the set of features and the target variable is not linear then we need to use polynomial regression of some degree
 - The degree of the polynomial is usually a hyperparameter of the model

Polynomial Regression



$$f(x) = w_1 x_1 + w_2 x_2 + w_3 x_3 + b$$

= $w_1(size) + w_2(size)^2 + w_3(size)^3 + b$

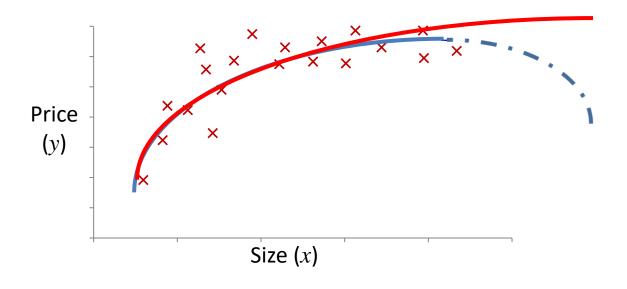
$$x_1 = (size)$$

$$x_2 = (size)^2$$

$$x_3 = (size)^3$$

- Polynomial regression is a special type of multiple regression whose independent variables are powers of variable X
- It is used to approximate a curve with unknown functional form
- For each additional power of X added to the model, the regression line will have one more bend

Polynomial Regression



$$f(x) = w_1(size) + w_2(size)^2 + b$$

$$f(x) = w_1(size) + w_2\sqrt{(size)} + b$$

Polynomial Regression

- The key observation here is that we can treat the powers of x: x, x^2 , ..., x^d , as distinct independent variables
 - Then, polynomial regression becomes a special case of multiple linear regression, since the model is still linear in the parameters that need to be estimated

 Therefore, we can find the optimal parameters w* using gradient descent

Feature Crosses

- A feature cross is a feature created by multiplying (crossing) two or more input features together. For example, x_1x_2 is a feature formed by multiplying the values of the features x_1 and x_2
 - Feature crosses can give our model better predictive abilities than just using the input features individually
- In a polynomial regression of degree d, we typically include the powers of all the input features up to degree d and all their possible combinations
 - For example, if we have two features and d = 2, then our new features will be: x_1 , x_2 , x_1x_2 , x_1^2 , x_2^2

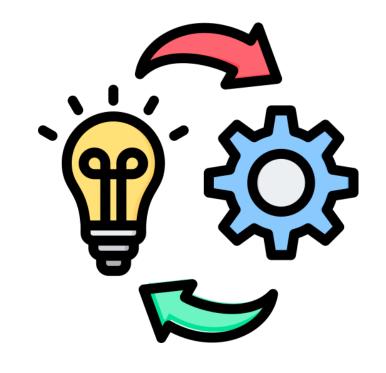
Polynomial Features

• For example, if we have two features and d = 2, then our new features will be: x_1 , x_2 , x_1x_2 , x_1^2 , x_2^2 , and the features matrix will be:

$$X = \begin{pmatrix} 1 & x_{11} & x_{12} & x_{11}x_{12} & x_{11}^2 & x_{12}^2 \\ 1 & x_{21} & x_{22} & x_{21}x_{22} & x_{21}^2 & x_{22}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & x_{n1}x_{n2} & x_{n1}^2 & x_{n2}^2 \end{pmatrix}$$

Scikit-learn provides the transformer
 <u>PolynomialFeatures</u> that creates the features matrix consisting of all the polynomial combinations of the features up to a specified degree

Regression Practical Considerations





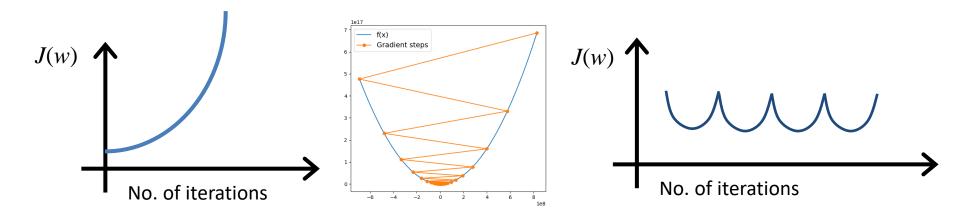
Gradient descent in practice:

- Debugging Learning rate
- Feature Scaling
- Regularization
- Regression Evaluation

Learning rate:

Gradient descent not working

Use smaller α



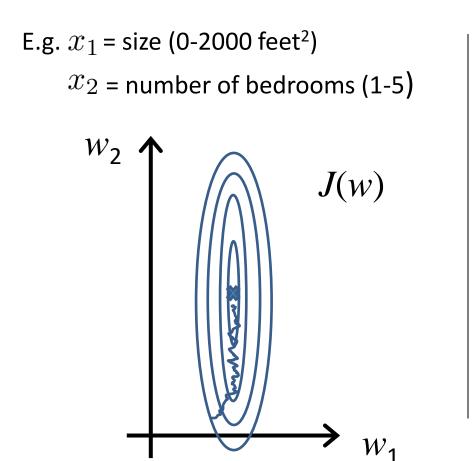
- For sufficiently small α , J(w) should decrease on every iteration
- If lpha is too small, gradient descent can be slow to converge
- If α is too large: J(w) may not decrease on every iteration; may not converge

To choose α , try

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

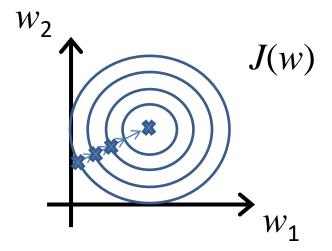
Feature Scaling: divide the input values by the range (i.e. the maximum value minus the minimum value) of the input variable, resulting in a new range of just 1.

The idea: Make sure features are on a similar scale. So that the gradient descent converges faster.



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

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



Rule-of-thumb: Get every feature into approximately a $-1 \le x_i \le 1$ range, $-0.5 \le x_i \le 0.5$, or other similar small ranges.

Mean normalization

• Replace x_i to make features have approximately zero mean (Do not apply to $x_0 = 1$):

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

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

$$x_1 = \frac{size - 1000}{2000}$$
 (average size of the houses is 1000, and ranges from 0 to 2000)

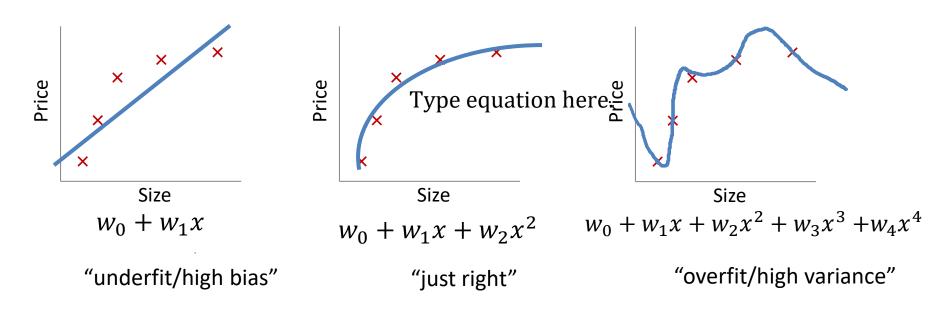
$$x_2 = \frac{\text{\#bedrooms}-2}{4}$$
 (average # of bedrooms is 2, and the range is from 1 to 5)

$$-0.5 \le x_1 \ge 0.5, -0.5 \le x_2 \ge 0.5,$$

Regularization

The problem of overfitting

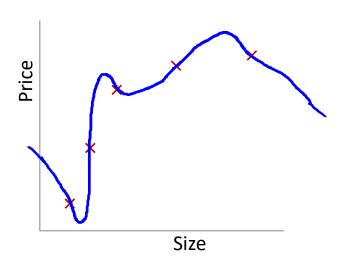
Example: Linear regression (housing prices)



Overfitting: If we have too many features, the learned hypothesis may fit the training set very well $\int_{i=1}^{\infty} \int_{i=1}^{\infty} (h_w(x^{(i)}) - y^{(i)})^2 \approx 0$) but fail to generalize to new examples (predict prices on new examples).

Addressing overfitting:

```
x_1 =  size of house x_2 =  no. of bedrooms x_3 =  no. of floors x_4 =  age of house x_5 =  average income in neighborhood x_6 =  kitchen size \vdots
```



Addressing overfitting:

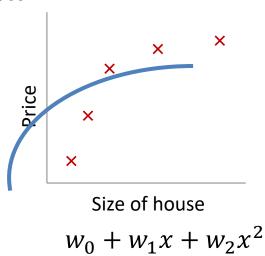
Options:

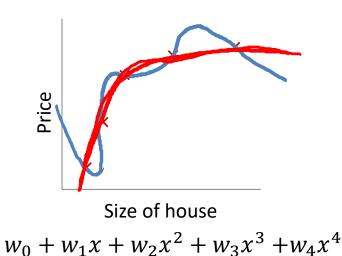
- 1. Reduce number of features.
 - Manually select which features to keep
 - Use feature selection algorithm
- 2. Regularization.
 - \circ Keep all the features, but reduce magnitude/values of parameters w_j
 - \circ Works well when we have a lot of features, each of which contributes a bit to predicting y

Regularization

Cost function

Intuition





Suppose we penalize and make w_3 , w_4 really small

$$J(w) = \frac{1}{2m} \sum_{i=1}^{m} (f_w(x^{(i)}) - y^{(i)})^2 + 1000 w_3^2 + 1000 w_4^2$$
$$w_3 \approx 0, \quad w_4 \approx 0$$

Regularization

Small values for parameters $w_1, w_2, ..., w_n$

- "Simpler/smoother" function
- Less prone to overfitting

Housing:

- Features: $x_1, x_2, ..., x_{100}$
- Parameters: $w_1, w_2, ..., w_{100}$

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

$$J(w) = \frac{1}{2m} \left[\sum_{i=1}^{m} (f_w(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} w_j^2 \right]$$

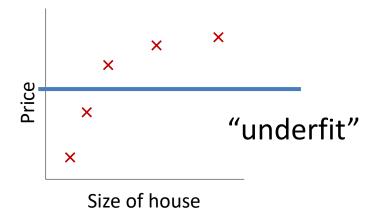
$$\min_{w} J(w)$$



In regularized linear regression, we choose w to minimize

$$J(w) = \frac{1}{2m} \left[\sum_{i=1}^{m} (f_w(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} w_j^2 \right]$$

What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda=10^{10}$)?



$$w_1x + w_2x^2 + w_3x^3 + w_4x^4 + b$$

$$w_1 \approx 0$$
, $w_2 \approx 0$, $w_3 \approx 0$, $w_4 \approx 0$

Regularized linear regression

$$J(w) = \frac{1}{2m} \left[\sum_{i=1}^{m} (f_w(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} w_j^2 \right]$$

$$\min_{w} J(w)$$

Gradient descent

Repeat {
$$w_0 = w_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (f_w(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$w_j = w_j - \alpha \left[\frac{1}{m} \sum_{i=1}^m (f_w(x^{(i)}) - y^{(i)}) x_j^{(i)} - \frac{\lambda}{m} w_j \right]$$

 $\frac{\partial}{\partial w_0}J(w)$

$$(j=\mathbf{x},1,2,3,\ldots,n)$$
 $\frac{\partial}{\partial w_j}J(w)$ "Regularized"

$$\{j = \mathbf{x}, 1, 2, 3, \dots, n\} \qquad \frac{\frac{\partial}{\partial w_j} J(w) \text{ "Regularized"}}{\frac{\partial}{\partial w_j} J(w) = w_j \left(1 - \alpha \frac{\lambda}{m}\right) - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(f_w(x^{(i)}) - y^{(i)}\right) x_j^{(i)}}$$

$$1 - \alpha \frac{\lambda}{m} < 1$$

Regression Evaluation

- Performance measured by
 - Mean Squared Error (MSE)

$$MSE = \frac{1}{n}\sum (y - \hat{y})^2$$

Root-Mean-Squared-Error (RMSE)

$$RMSE = \sqrt{\frac{(y - \hat{y})^2}{n}}$$

Mean-Absolute-Error (MAE)

$$MAE = \frac{1}{n} \sum |y - \widehat{y}|$$

...others