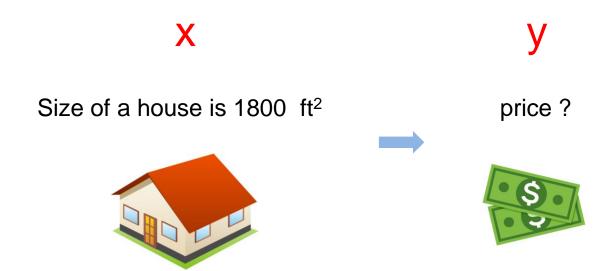


Regression, Gradient Descent

Machine Learning (PM chap 2, 10)

Regression

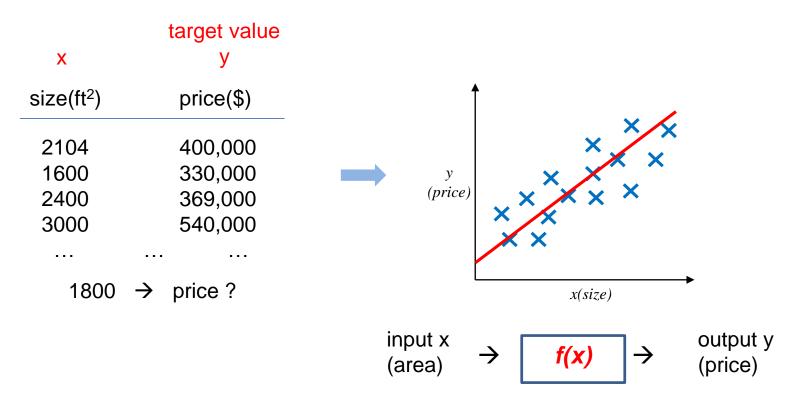
■ From $x \rightarrow$ predict y



Regression

Predicting value y

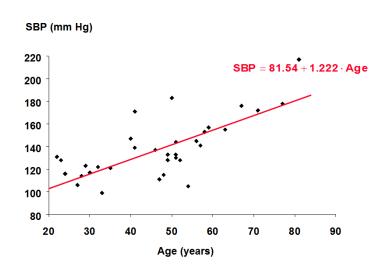
- From x (input value) → predict y (output/target value, continuous)
- Regression: constructing a model y = f(x), using training data (x, y)

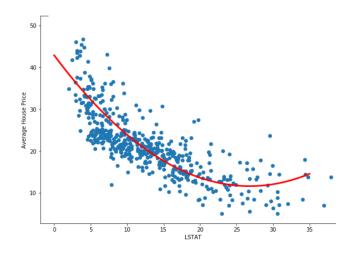


Regression

Examples

- Age vs. Blood pressure
- Lower status % vs. House price



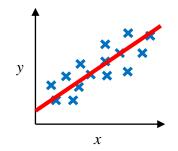


Linear Regression

- The model
 - y = f(x) is modeled as a linear function

$$y = f_{\theta}(x) = w \cdot x + b$$

parameters
(w, b)



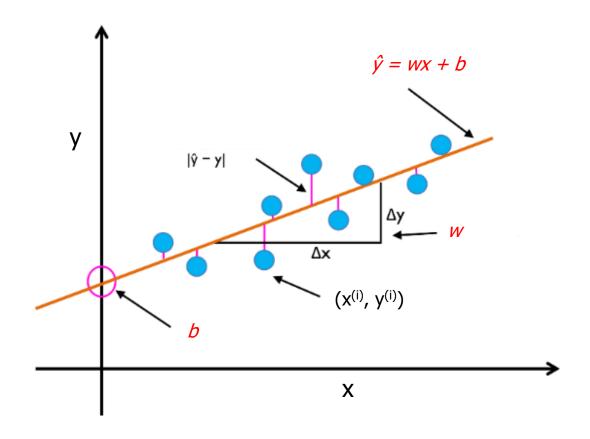
X	У
2104	400
1600	330
2400	369
3000	540

- w and b are estimated using the training data $(x^{(i)}, y^{(i)})$
 - w : weight (coefficient)
 - b : bias (intercept)

- θ : parameters
- Minimize prediction error \rightarrow find w and b
 - Least square method
 - Gradient descent

Estimating Parameters

- Finding optimal w, b
 - Minimize the difference between actual value y and predicted value \hat{y}



Cost Function

- Cost(loss) function
 - A measure of how wrong the model is in terms of its ability to estimate the relationship between x and y
 - Goal of learning is to minimize the cost function
- Data

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})$$

Prediction model

$$\hat{y} = f_{\theta}(x)$$

MSE(mean square error) cost function

$$J(\boldsymbol{\theta}) = \frac{1}{2m} \sum_{i} (\hat{y}^{(i)} - y^{(i)})^{2} = \frac{1}{2m} \sum_{i} (f_{\theta}(x^{(i)}) - y^{(i)})^{2}$$

- Gradient descent
 - An iterative method for finding parameters to minimize a function Goal: $\min_{\theta} J(\theta)$
- Gradient
 - Gradient of a multivariate function
 - = vector of derivatives (slopes)

$$\nabla J(\theta) = \left(\frac{\partial J}{\partial \theta_0}, \frac{\partial J}{\partial \theta_1}, \dots, \frac{\partial J}{\partial \theta_m}\right)$$

= direction of fastest increase

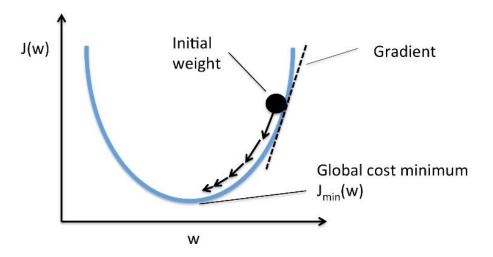
- Takes steps proportional to the negative of the gradient
- If the model has 1 parameter w,
 - Repeat

If
$$\frac{\partial J}{\partial w} > 0 \rightarrow \text{decrease w}$$

 $\frac{\partial J}{\partial w} < 0 \rightarrow \text{increase w}$

$$\therefore \qquad w = w - \alpha \frac{\partial J}{\partial w}$$

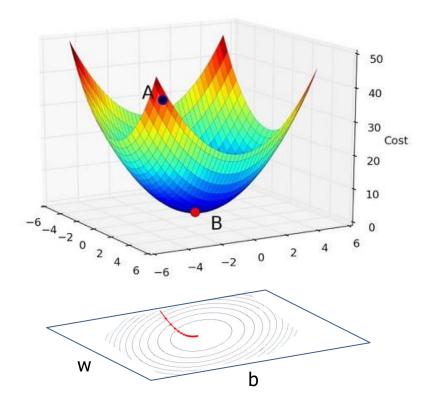
 α : learning rate



- If the model has parameters w and b,
 - Repeat

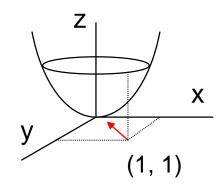
$$w = w - \alpha \frac{\partial J}{\partial w}$$

$$b = b - \alpha \frac{\partial J}{\partial b}$$



Example

• Function
$$z = f(x, y) = x^2 + y^2$$



Gradient
$$\left(\frac{\partial f}{\partial x} = 2x, \frac{\partial f}{\partial y} = 2y\right)$$

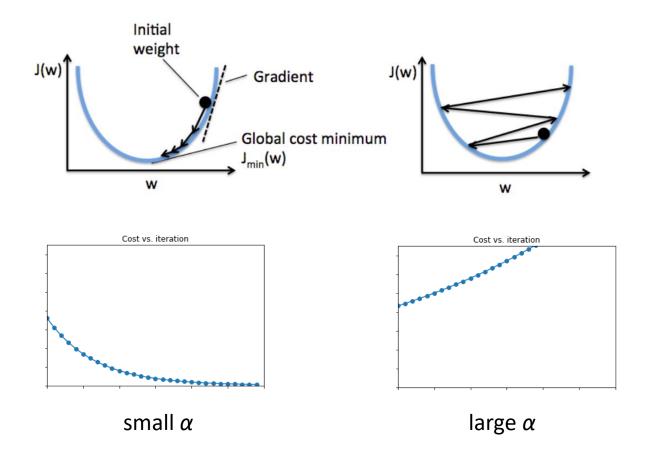
- At $(x=1, y=1) \rightarrow gradient is (2, 2)$
 - \therefore The direction that most rapidly reduce z is (-2, -2)
- For $\alpha = 0.1$,

$$x = x - \alpha \cdot \frac{\partial f}{\partial x} = 1 - 0.1 \cdot 2 = 0.8$$

$$y = y - \alpha \cdot \frac{\partial f}{\partial y} = 1 - 0.1 \cdot 2 = 0.8$$

Learning Rate

• Effect of learning rate α



GD for Linear Regression

Data
$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})$$

• Model
$$\hat{y} = wx + b$$

• Cost
$$J(w,b) = \frac{1}{2m} \sum (\hat{y}^{(i)} - y^{(i)})^2$$

Gradients

$$\frac{\partial J}{\partial w} = \frac{\partial}{\partial w} \frac{1}{2m} \sum_{i} (\hat{y}^{(i)} - y^{(i)})^2 = \frac{1}{m} \sum_{i} (\hat{y}^{(i)} - y^{(i)}) \frac{\partial}{\partial w} (wx^{(i)} + b)$$
$$= \frac{1}{m} \sum_{i} (\hat{y}^{(i)} - y^{(i)}) x^{(i)}$$

$$\frac{\partial J}{\partial b} = \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)})$$

GD for Linear Regression

Learning (gradient descent)

Given
$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(m)}, y^{(m)})$$

Initialize w, b

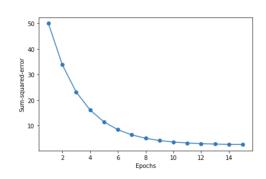
Repeat

$$\hat{y}^{(i)} = wx^{(i)} + b$$

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

$$w = w - \alpha \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)}) x^{(i)}$$
$$b = b - \alpha \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)})$$

$$cost = \frac{1}{2m} \sum (\hat{y}^{(i)} - y^{(i)})^2$$

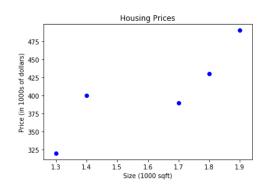


Data

```
x_train = np.array([1.8, 1.3, 1.7, 1.9, 1.4])
y_train = np.array([430., 320., 390., 490., 400.])
```

• Compute \hat{y} and cost

Compute gradient



$$\hat{y} = wx + b$$

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

$$\frac{\partial J}{\partial w} = \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)}) x^{(i)}$$
$$\frac{\partial J}{\partial b} = \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)})$$

Learning (gradient descent)

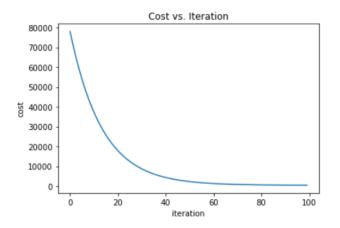
```
def gradient_descent(x, y, w, b, alpha, num_iters):
    J_history = []
    for i in range(num_iters):
        dj_dw, dj_db = compute_gradient(x, y, w, b)
        w = w - alpha * dj_dw
        b = b - alpha * dj_db
        J history.append(compute cost(x, y, w, b))
        b = b - \alpha \frac{\partial J}{\partial b}
```

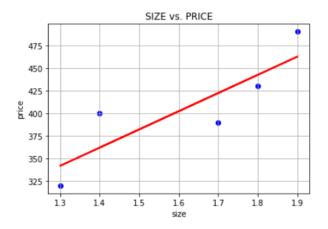
Cost change

```
plt.plot(J_hist[:100])
```

Learned model

```
y_hat = predict(x_train, w_final, b_final)
plt.plot(x_train, y_hat, color='red')
```

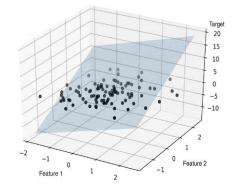




Multiple Linear Regression

- The model
 - y = f(x) is modeled as a linear function

$$y = f_{\theta}(x) = W_0 \cdot X_0 + W_1 \cdot X_1 + b$$
parameters
(W_0, W_1, b)



x0	x1	у
2104	4	400
1600	2	330
2400	3	369
3000	5	540

- w_0 , w_1 and b are estimated using the training data ($x^{(i)}$, $y^{(i)}$)
 - w_0, w_1 : weight (coefficient) θ : parameters
 - b: bias (intercept)

Data
$$(x_0^{(1)}, x_1^{(1)}, \dots, y^{(1)}), (x_0^{(2)}, x_1^{(2)}, \dots, y^{(2)}), \dots, (x_0^{(m)}, x_1^{(m)}, \dots, y^{(m)})$$

• Model
$$\hat{y} = w_0 x_0 + w_1 x_1 + \dots + b$$

Cost
$$J(\boldsymbol{\theta}) = \frac{1}{2m} \sum_{i} (\hat{y}^{(i)} - y^{(i)})^2$$

Gradients

$$\frac{\partial J}{\partial w_0} = \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)}) x_0^{(i)}$$
$$\frac{\partial J}{\partial w_1} = \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)}) x_1^{(i)}$$
...

$$\frac{\partial J}{\partial b} = \frac{1}{m} \sum (\hat{y}^{(i)} - y^{(i)})$$

Vector form - Data (N features, M data)

$$\mathbf{X} = \begin{bmatrix} x_0^{(1)} & x_1^{(1)} & \dots \\ x_0^{(2)} & x_1^{(2)} & \dots \\ x_0^{(3)} & x_1^{(3)} & \dots \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \dots \end{bmatrix}$$

$$(N \times 1)$$

Model

$$\hat{y}^{(1)} = w_0 x_0^{(1)} + w_1 x_1^{(1)} \dots + b$$

$$\hat{y}^{(2)} = w_0 x_0^{(2)} + w_1 x_1^{(2)} \dots + b$$

$$\hat{y}^{(3)} = w_0 x_0^{(3)} + w_1 x_1^{(3)} \dots + b$$
...

Cost

$$J(\theta) = \frac{1}{2m} \sum_{i} (\hat{y}^{(i)} - y^{(i)})^2$$

$$\begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \hat{y}^{(3)} \end{bmatrix} = \begin{bmatrix} x_0^{(1)} & x_1^{(1)}, \dots \\ x_0^{(2)} & x_1^{(2)}, \dots \\ x_0^{(3)} & x_1^{(3)}, \dots \end{bmatrix} \cdot \begin{bmatrix} w_0 \\ w_1 \\ \dots \end{bmatrix} + b$$

$$\hat{\mathbf{v}} = \mathbf{X}\mathbf{w} + b$$

$$cost = \frac{1}{2m} sum(\hat{\mathbf{y}} - \mathbf{y})^{2}$$
$$((\mathbf{X}\mathbf{w} + b - \mathbf{y})^{T} (\mathbf{X}\mathbf{w} + b - \mathbf{y}))$$

Gradient

$$\frac{\partial J}{\partial w_0} = \frac{1}{m} \left((\hat{y}^{(1)} - y^{(1)}) x_0^{(1)} + (\hat{y}^{(2)} - y^{(2)}) x_0^{(2)} + \cdots \right)$$

$$\frac{\partial J}{\partial w_1} = \frac{1}{m} \left((\hat{y}^{(1)} - y^{(1)}) x_1^{(1)} + (\hat{y}^{(2)} - y^{(2)}) x_1^{(2)} + \cdots \right)$$
...

$$\frac{\partial J}{\partial b} = \frac{1}{m} \left((\hat{y}^{(1)} - y^{(1)}) + (\hat{y}^{(2)} - y^{(2)}) + \cdots \right)$$

$$\frac{\partial J}{\partial w_0} = \frac{1}{m} \left((\hat{y}^{(1)} - y^{(1)}) x_0^{(1)} + (\hat{y}^{(2)} - y^{(2)}) x_0^{(2)} + \cdots \right) \qquad \left[\frac{\partial J}{\partial w_0} \right] = \frac{1}{m} \left[x_0^{(1)}, x_0^{(2)}, x_0^{(3)}, \dots \right] \cdot \begin{bmatrix} \hat{y}^{(1)} - y^{(1)} \\ \hat{y}^{(2)} - y^{(2)} \\ \hat{y}^{(3)} - y^{(3)} \end{bmatrix} = \frac{1}{m} \begin{bmatrix} x_0^{(1)}, x_0^{(2)}, x_0^{(3)}, \dots \\ x_1^{(1)}, x_1^{(2)}, x_1^{(3)}, \dots \end{bmatrix} \cdot \begin{bmatrix} \hat{y}^{(1)} - y^{(1)} \\ \hat{y}^{(2)} - y^{(2)} \\ \hat{y}^{(3)} - y^{(3)} \end{bmatrix} = \frac{1}{m} \begin{bmatrix} x_0^{(1)}, x_0^{(2)}, x_0^{(3)}, \dots \\ x_1^{(1)}, x_1^{(2)}, x_1^{(3)}, \dots \end{bmatrix} \cdot \begin{bmatrix} \hat{y}^{(1)} - y^{(1)} \\ \hat{y}^{(2)} - y^{(2)} \\ \hat{y}^{(3)} - y^{(3)} \end{bmatrix}$$

$$\nabla J(\mathbf{w}) = \frac{1}{m} \mathbf{X}^{\mathsf{T}} (\hat{\mathbf{y}} - \mathbf{y})$$

$$\frac{\partial J}{\partial b} = \frac{1}{m} \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} \hat{y}^{(1)} - y^{(1)} \\ \hat{y}^{(2)} - y^{(2)} \\ \hat{y}^{(3)} - y^{(3)} \end{bmatrix}$$

$$\frac{\partial J}{\partial b} = \frac{1}{m} sum(\hat{\mathbf{y}} - \mathbf{y})$$

Learning (gradient descent)

Given

$$\mathbf{X} = \begin{bmatrix} x_0^{(1)} & x_1^{(1)} & \dots \\ x_0^{(2)} & x_1^{(2)} & \dots \\ x_0^{(3)} & x_1^{(3)} & \dots \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \dots \end{bmatrix}$$

$$\mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \dots \end{bmatrix}$$

Initialize
$$\mathbf{w} = [w_1 \ w_2 \ ...], b$$

repeat

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} + b$$

$$\mathbf{w} = \mathbf{w} - \alpha \frac{1}{m} (\mathbf{X}^{\mathsf{T}} (\hat{\mathbf{y}} - \mathbf{y}))$$

$$\mathbf{w} = \mathbf{w} - \alpha \nabla J(\mathbf{w})$$

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

$$b = b - \alpha \frac{\partial J}{\partial b}$$

$$\mathbf{w} = \mathbf{w} - \alpha \, \nabla J(\mathbf{w})$$

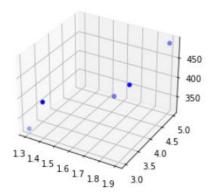
$$b = b - \alpha \frac{\partial J}{\partial b}$$

$$cost = \frac{1}{2m} sum(\hat{\mathbf{y}} - \mathbf{y})^2$$

Data

```
X_{\text{train}} = \text{np.array}([[1.8, 4], [1.3, 3], [1.7, 4], [1.9, 5], [1.4, 3]])

y_{\text{train}} = \text{np.array}([430., 320., 390., 490., 400.])
```



• Compute \hat{y} and cost

Compute gradients

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} + b$$

$$cost = \frac{1}{2m}sum(\hat{\mathbf{y}} - \mathbf{y})^2$$

$$\frac{\partial J}{\partial \mathbf{w}} = \frac{1}{m} \mathbf{X}^{\mathsf{T}} (\hat{\mathbf{y}} - \mathbf{y})$$
$$\frac{\partial J}{\partial b} = \frac{1}{m} sum(\hat{\mathbf{y}} - \mathbf{y})$$

Learning (gradient descent)

```
def gradient_descent(X, y, w, b, alpha, num_iters):
    J_history = []
    for i in range(num_iters):
        dj_dw, dj_db = compute_gradient(X, y, w, b)

        w = w - alpha * dj_dw
        b = b - alpha * dj_db

        J_history.append(compute_cost(X, y, w, b))
w = w - \alpha \nabla J(w)
b = b - \alpha \frac{\partial J}{\partial b}
```

Cost change

```
Plt.plot(J_hist[:100])

Cost vs. Iteration

Fig. 30000

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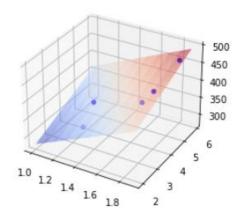
10000

10
```

Learned model

```
fig, ax = plt.subplots(subplot_kw={"projection": "3d"})
ax.scatter(X_train[:,0], X_train[:,1], y_train, marker='o', c='blue')
X = np.arange(1, 2, 0.1)
Y = np.arange(2, 6, 0.1)
X, Y = np.meshgrid(X, Y)

Z = w_final[0]*X + w_final[1]*Y + b_final
ax.plot_surface(X, Y, Z, cmap=cm.coolwarm, alpha=0.5)
```



Different notation

Different notation (ex> Python ML book)

$$\mathbf{x} = \begin{bmatrix} x_0 & x_1 \end{bmatrix}$$

$$\mathbf{w} = \begin{bmatrix} w_0 & w_1 \end{bmatrix}, \qquad b$$

$$\hat{y} = w_0 x_0 + w_1 x_1 + b$$

$$\mathbf{X} = \begin{bmatrix} x_0^{(1)} & x_1^{(1)} \\ x_0^{(2)} & x_1^{(2)} \\ x_0^{(3)} & x_1^{(3)} \end{bmatrix}$$
...

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} + b$$

$$\mathbf{x} = [1 \quad x_1 \quad x_2]$$
 $\mathbf{w} = [w_0 \quad w_1 \quad w_2] \quad (w_0 = b)$
 $\hat{y} = w_0 + w_1 x_1 + w_2 x_2$

$$\mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} \\ 1 & x_1^{(3)} & x_2^{(3)} \end{bmatrix}$$
...

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w}$$

Closed Form Solution

Cost function

$$J(\mathbf{w}) = \|\hat{\mathbf{y}} - \mathbf{y}\|^2 = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y})$$

Minimize w

$$\|\mathbf{y}\| = \left(\sum (y^{(i)})^2\right)^{\frac{1}{2}}$$

$$\frac{\partial J}{\partial \mathbf{w}} = 2 \mathbf{X}^{\mathsf{T}} (\mathbf{X} \mathbf{w} - \mathbf{y}) = \mathbf{0}$$

$$\mathbf{X}^{\mathbf{T}}\mathbf{X}\mathbf{w} = \mathbf{X}^{\mathbf{T}}\mathbf{y}$$

$$\therefore \mathbf{w} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{y}$$

Solving w using normal equation

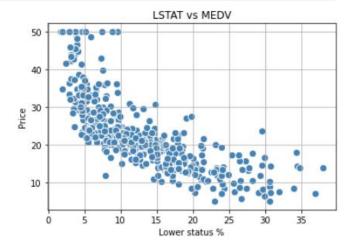
- Only for linear regression can not be applied to other learning algorithms
- Solving the normal equation can be very difficult for large N and M

Linear Regression using Scikit Learn

The Boston housing dataset

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	В	LSTAT	MEDV
0	0.00632	18.0	2.31	0	0.538	6.575	65.2	4.0900	1	296.0	15.3	396.90	4.98	24.0
1	0.02731	0.0	7.07	0	0.469	6.421	78.9	4.9671	2	242.0	17.8	396.90	9.14	21.6
2	0.02729	0.0	7.07	0	0.469	7.185	61.1	4.9671	2	242.0	17.8	392.83	4.03	34.7
3	0.03237	0.0	2.18	0	0.458	6.998	45.8	6.0622	3	222.0	18.7	394.63	2.94	33.4
4	0.06905	0.0	2.18	0	0.458	7.147	54.2	6.0622	3	222.0	18.7	396.90	5.33	36.2

- RM average number of rooms per dwelling
- LSTAT percentage of lower status of the population
- MEDV median value of owner-occupied homes



Linear Regression using Scikit Learn

Use sklearn.linear_model.LinearRegression. Training the model - .fit()

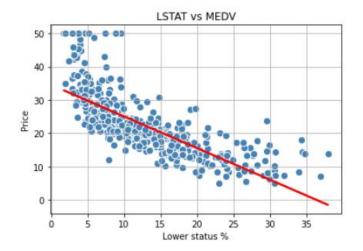
```
from sklearn.linear_model import LinearRegression
# training the model
lr = LinearRegression()
lr.fit(X, y)
```

```
# model parameters
print('w = ', lr.coef_)
print('b = ', lr.intercept_)

w = [[ 9.10210898]]
b = [-34.67062078]
```

Predicting values - .predict()

```
y_hat = lr.predict(X)
# print the MSE
print('MSE : %.2f' % mean_squared_error(y, y_hat))
MSF : 38.48
```

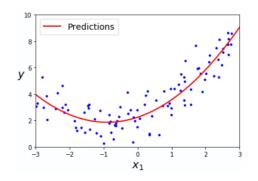


Polynomial Regression

- The model
 - y = f(x) is modeled as a polynomial function

$$y = f_{\theta}(x) = w_0 \cdot x + w_1 \cdot x^2 + w_2 \cdot x^3 + \dots + b$$

parameters
 (w_0, w_1, b)



- We can use multiple linear regression
 - Introduce new features
 - Data

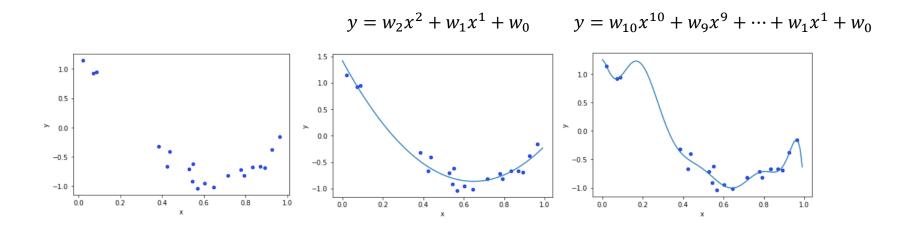
$$(x,y) \longrightarrow (x,x^2,x^3,...,y)$$

Model

$$\hat{y} = w_0 x + w_1 x^2 + \dots + b$$

Regularization

- Overfitting
 - When the model is too complex
 - → good for training data, but bad for test data
- Example

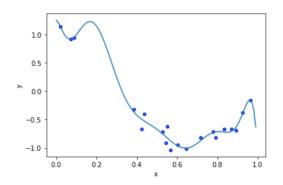


Regularization

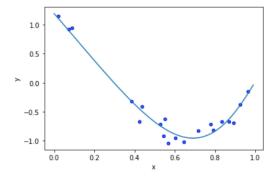
Regularization

- Reduce the size of parameters w
 - → make the model simpler
- Example

$$y = w_{10}x^{10} + w_9x^9 + \dots + w_1x^1 + w_0$$



$$y = w_{10}x^{10} + w_9x^9 + \dots + w_1x^1 + w_0$$



Regularization

- How to reduce w?
 - Add regularization term(penalty) to a cost function

Ex>
$$Cost Function = J(w) + \frac{1}{2m} \lambda \sum_{j=1}^{n} w_j^2$$

- λ : regularization parameter
- Then, minimizing cost = reduce $w \rightarrow reduce$ complexity
- Gradient descent

$$w_j = w_j - \alpha \frac{\partial J}{\partial w_i} - \alpha \frac{\lambda}{m} w_j$$

If $\lambda=0$, the model overfits $(y=w_{10}x^{10}+w_9x^9+\cdots+w_1x^1+w_0)$ If λ is too large, the model underfits $(y=w_1x^1+w_0)$

Polynomial Regression using Scikit Learn

- Extending $x \rightarrow x$, x^2 , x^3 , ...
 - sklearn.preprocessing.PolynomialFeatures

- Regularizing linear regression
 - sklearn.linear_model.Ridge
 - Cost = $\|\mathbf{X}\mathbf{w} \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2$
 - 'alpha' is the regularization parameter

Polynomial Regression using Scikit Learn

- Data
 - (x, cos(x)+random noise)
- Polynomial regression with degree=10

```
lr = LinearRegression()
lr.fit(X_poly, y)

X_test = np.arange(0, 1, 0.01).reshape(-1, 1)
X_test_poly = poly.fit_transform(X_test)

plt.plot(X_test, lr.predict(X_test_poly))
```

• Regularization – use Ridge with λ

```
lr = Ridge(alpha = 0.01)
lr.fit(X_poly, y)

X_test = np.arange(0, 1, 0.01).reshape(-1, 1)
X_test_poly = poly.fit_transform(X_test)

plt.plot(X_test, lr.predict(X_test_poly))
```

