# Day 3: Overfitting and Generalization

## Summer STEM: Machine Learning

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# Outline

# Review

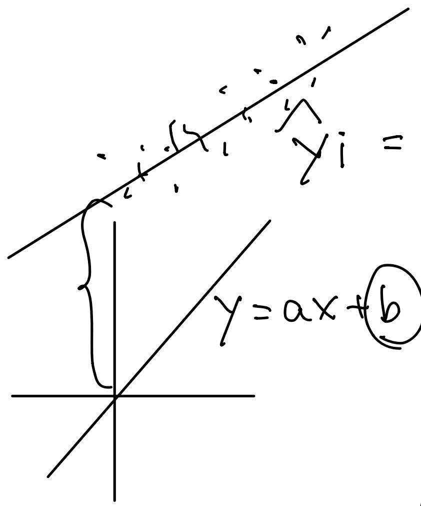
- For the Boston housing dataset we have the following information in the data:
- ‘CRIM’,‘ZN’,‘INDUS’,‘CHAS’,‘NOX’,‘RM’,‘AGE’,‘DIS’, ‘RAD’,‘TAX’,‘PTRATIO’,‘B’,‘LSTAT’,‘PRICE’
- What is the feature and label if we want to estimate price?
- What is the feature and label if we want to estimate RM? (RM: average number of rooms per dwelling)

# Review

- You have a bunch of photos of 6 people but without information about who is on which one and you want to divide this dataset into 6 piles, each with the photos of one individual.
- You have a bunch of molecules and information about which are drugs and you train a model to answer whether a new molecule is also a drug.
- (Credit to lejlot)

# Review

- You have a large inventory of identical items, you want to predict how many you can sell in the next 3 months.
- You want a software to examine individual costumer's account and for each account decide if it has been hacked.
- (Credit to Andrew Ng)




$\hat{y}_i = w_1 x_i + w_0$

bias
intercept

Loss: $\frac{1}{N}\sum_{i=1}^{N} \|y_i - \hat{y}_i\|^2 = \|Y - Xw\|$

$$W_0 + W_1 X_i$$

$$= W_0 \cdot 1 + W_1 \cdot X_i =$$

$$= \underset{1\times 2}{\begin{bmatrix} 1 & X_i \end{bmatrix}} \cdot \underset{2\times 1}{\begin{bmatrix} W_0 \\ W_1 \end{bmatrix}}$$

$N = 10{,}000$

$$\frac{1}{N}\sum_{i=1}^{N} \|y_i - \hat{y}_i\|^2$$

$$= \frac{1}{N}\left(\|y_1 - \hat{y}_1\|^2 + \|y_2 - \hat{y}_2\|^2 + \cdots + \|y_N - \hat{y}_N\|^2\right)$$

$a$

sum = 0
for i in (1-N)

sum = sum $+ \|y_i - \hat{y}_i\|^2$

sum = $\frac{1}{N}$ * sum

$$\frac{1}{N}\|Y - Xw\|^2$$

$$(\sqrt{a^2})^2 = a^2$$

$N \times 3$ $\quad 3 \times 1$

$$= \frac{1}{N}\left\| \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} 1 & x_{11} & x_{12} \\ 1 & x_{21} & x_{22} \\ & \vdots & \\ 1 & x_{N1} & x_{N2} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} \right\|^2$$

$$= \frac{1}{N}\left\| \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} w_0 + w_1 x_{11} + w_2 x_{12} \\ w_0 + w_1 x_{21} + w_2 x_{22} \\ \vdots \\ w_0 + w_1 x_{N1} + w_2 x_{N2} \end{bmatrix} \right\|^2$$

$$= \frac{1}{N}\left\| \begin{bmatrix} y_1 - (w_0 + w_1 x_{11} + w_2 x_{12}) \\ y_2 - (w_0 + w_1 x_{21} + w_2 x_{22}) \\ \vdots \\ y_N - (w_0 + w_1 x_{N1} + w_2 x_{N2}) \end{bmatrix} \begin{matrix} \hat{y}_1 \\ \hat{y}_2 \\ \\ \hat{y}_N \end{matrix} \right\|^2$$

$$= \frac{1}{n} \left\| \begin{bmatrix} y_1 - \hat{y}_1 \\ y_2 - \hat{y}_2 \\ \vdots \\ y_n - \hat{y}_n \end{bmatrix} \right\|^2$$

$$\left\| \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right\| = \sqrt{y_1^2 + y_2^2 + y_3^2}$$

$$= \frac{1}{n} \left( (y_1 - \hat{y}_1)^2 + (y_2 - y_2)^2 + \cdots + (y_n - \hat{y}_n)^2 \right)$$

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$$(X^T X)^{-1} X^T Y = w$$

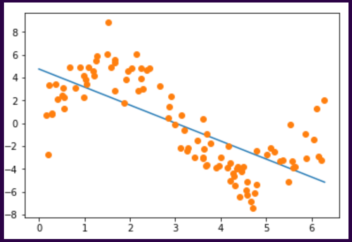
$$Y = Xw$$

$$X^{-1} Y = X^{-1} X w = w$$

# Outline

# Polynomial Fitting

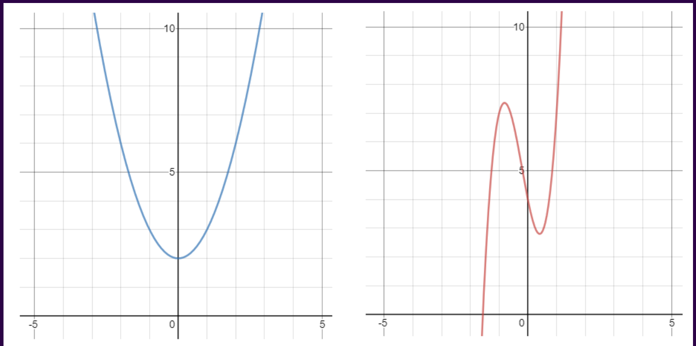
- We have been using straight lines to fit our data. But it doesn't work well every time
- Some data have more complex relation that cannot be fitted well using a straight line




- Can we use some other model to fit this data?

# Polynomial Fitting

- Can we use a polynomial to fit our data?
- Polynomial: A sum of different powers of a variable
  - Examples: $y = x^2 + 2$, $y = 5x^3 - 3x^2 + 4$



# Polynomial Fitting

- Polynomials of $x$: $\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \cdots + w_M x^M$
- $M$ is called the order of the polynomial.
- The process of fitting a polynomial is similar to linearly fitting multivariate data.

# Polynomial fitting

- Rewrite in matrix-vector form

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \approx \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^M \\ 1 & x_2 & x_2^2 & \cdots & x_2^M \\ \vdots & & \ddots & & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^M \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_M \end{bmatrix}$$

- This can still be written as

  $Y \approx X\mathbf{w}$

- Loss $J(\mathbf{w}) = \frac{1}{N}\|Y - X\mathbf{w}\|^2$
- The i-th row of the design matrix $X$ is simply a transformed feature $\phi(x_i) = (1, x_i, x_i^2, \cdots, x_i^M)$

# Polynomial Fitting

- Original design matrix: $\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix}$
- Design matrix after feature transformation:
$$\begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^M \\ 1 & x_2 & x_2^2 & \cdots & x_2^M \\ \vdots & & \ddots & & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^M \end{bmatrix}$$
- For the polynomial fitting, we just added columns of features that are powers of the original feature

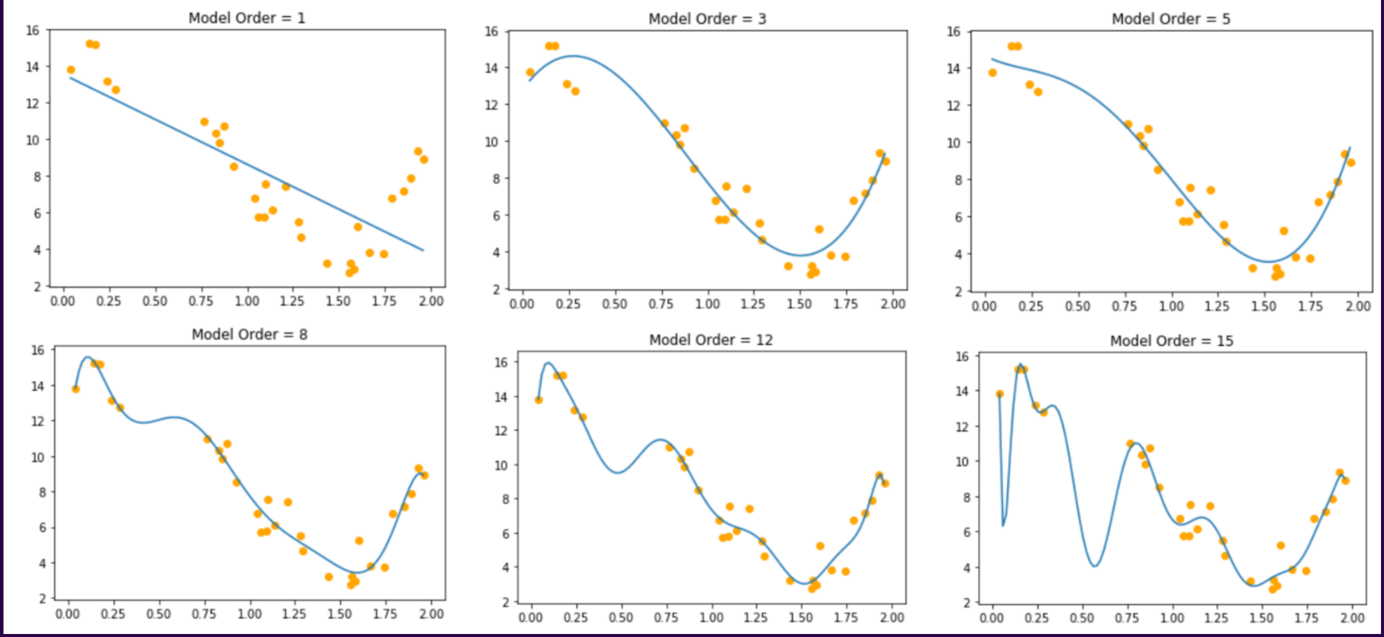
# Linear Regression

- Model $\hat{y} = \mathbf{w}^T \phi(\mathbf{x})$
- Loss $J(\mathbf{w}) = \dfrac{1}{N} \|Y - X\mathbf{w}\|^2$
- Find $\mathbf{w}$ that minimizes $J(\mathbf{w})$

# Overfitting

- We learned how to fit our data using polynomials of different order
- With a higher model order, we can fit the data with increasing accuracy
- As you increase the model order, at certain point it is possible find a model that fits your data perfectly (ie. zero error)
- What could be the problem?

# Overfitting



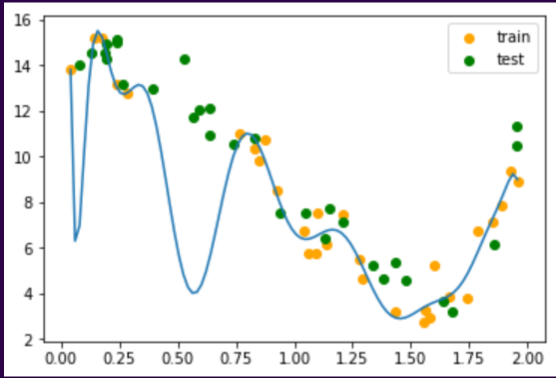

- Which of these model do you think is the best? Why?

# Demo

Open demo_fit_polynomial.ipynb

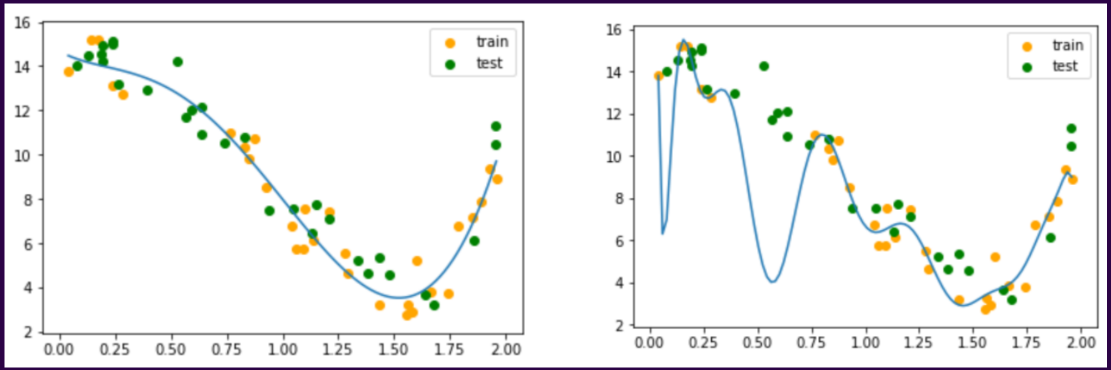
# Overfitting

- The problem is that we are only fitting our model using data that is given
- Data usually contains noise
- When a model becomes too complex, it will start to fit the noise in the data
- What happens if we apply our model to predict some data that the model has never seen before? It will not work well.
- This is called over-fitting



# Overfitting

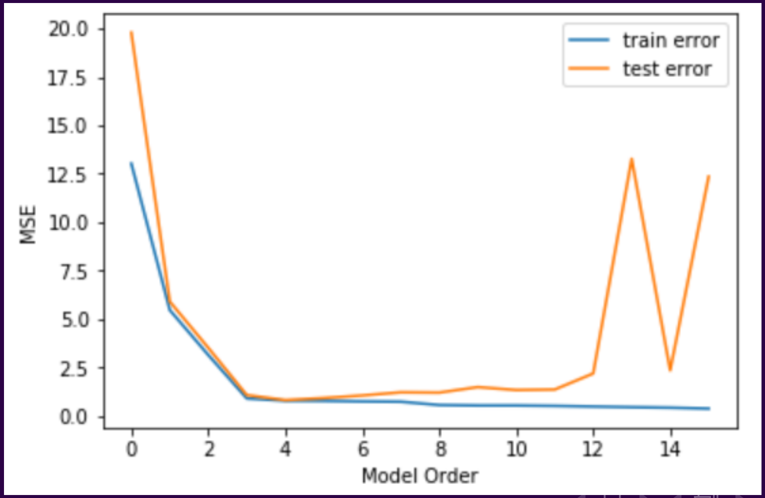
- Split the data set into a train set and a test set
- Train set will be used to train the model
- The test set will not be seen by the model during the training process
- Use test set to evaluate the model when a model is trained




- With the training and test sets shown, which one do you think is the better model now?

# Train and Test Error

- Plot of train error and test error for different model order
- Initially both train and test error go down as model order increase
- But at a certain point, test error start to increase because of overfitting



# Outline

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# How can we prevent overfitting without knowing the model order before-hand?

- **Regularization**: methods to prevent overfitting
  - We just covered regularization by model order selection
- Is there another way? Talk among your classmates.
  - Solution: We can change our cost function.

# Weight Based Regularization

- Looking back at the polynomial overfitting
- Notice that weight-size increases with overfitting

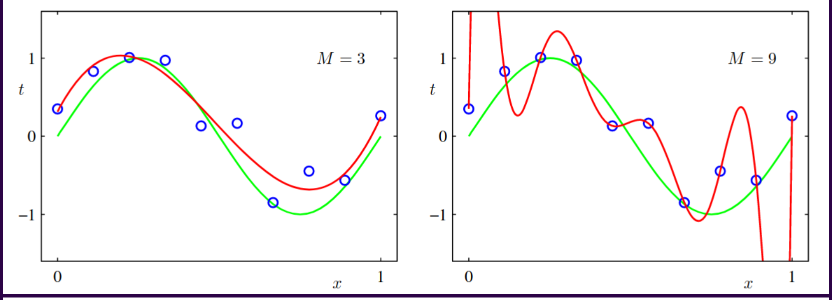


**Table 1.1** Table of the coefficients $\mathbf{w}^\star$ for polynomials of various order. Observe how the typical magnitude of the coefficients increases dramatically as the order of the polynomial increases.

| | $M=0$ | $M=1$ | $M=6$ | $M=9$ |
|---|---|---|---|---|
| $w_0^\star$ | 0.19 | 0.82 | 0.31 | 0.35 |
| $w_1^\star$ | | -1.27 | 7.99 | 232.37 |
| $w_2^\star$ | | | -25.43 | -5321.83 |
| $w_3^\star$ | | | 17.37 | 48568.31 |
| $w_4^\star$ | | | | -231639.30 |
| $w_5^\star$ | | | | 640042.26 |
| $w_6^\star$ | | | | -1061800.52 |
| $w_7^\star$ | | | | 1042400.18 |
| $w_8^\star$ | | | | -557682.99 |
| $w_9^\star$ | | | | 125201.43 |

# New Cost Function

$$J(\mathbf{w}) = \frac{1}{N} \|Y - X\mathbf{w}\|^2 + \lambda \|\mathbf{w}\|^2$$

- Penalize complexity by simultaneously minimizing weight values.
- We call $\lambda$ a **hyper-parameter**
  - $\lambda$ determines relative importance

**Table 1.2** Table of the coefficients $\mathbf{w}^\star$ for $M = 9$ polynomials with various values for the regularization parameter $\lambda$. Note that $\ln\lambda = -\infty$ corresponds to a model with no regularization, i.e., to the graph at the bottom right in Figure 1.4. We see that, as the value of $\lambda$ increases, the typical magnitude of the coefficients gets smaller.

| | $\ln\lambda = -\infty$ | $\ln\lambda = -18$ | $\ln\lambda = 0$ |
|---|---|---|---|
| $w_0^\star$ | 0.35 | 0.35 | 0.13 |
| $w_1^\star$ | 232.37 | 4.74 | -0.05 |
| $w_2^\star$ | -5321.83 | -0.77 | -0.06 |
| $w_3^\star$ | 48568.31 | -31.97 | -0.05 |
| $w_4^\star$ | -231639.30 | -3.89 | -0.03 |
| $w_5^\star$ | 640042.26 | 55.28 | -0.02 |
| $w_6^\star$ | -1061800.52 | 41.32 | -0.01 |
| $w_7^\star$ | 1042400.18 | -45.95 | -0.00 |
| $w_8^\star$ | -557682.99 | -91.53 | 0.00 |
| $w_9^\star$ | 125201.43 | 72.68 | 0.01 |

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# Tuning Hyper-parameters

- Motivation: never determine a hyper-parameter based on training data
- **Hyper-Parameter**: a parameter of the algorithm that is not a model-parameter solved for in optimization.
  - Ex: $\lambda$ weight regularization value vs. model weights ($\mathbf{w}$)
- Solution: split dataset into three
  - **Training set**: to compute the model-parameters ($\mathbf{w}$)
  - **Validation set**: to tune hyper-parameters ($\lambda$)
  - **Test set**: to compute the performance of the algorithm (MSE)

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# Demo

Open demo_overfitting_regularization.ipynb

# Outline

# Motivation

- Cannot rely on closed form solutions
  - Computation efficiency: operations like inverting a matrix is not efficient
  - For more complex problems such as neural networks, a closed-form solution is not always available
- Need an optimization technique to find an optimal solution
  - Machine learning practitioners use **gradient**-based methods

# Gradient Descent Algorithm

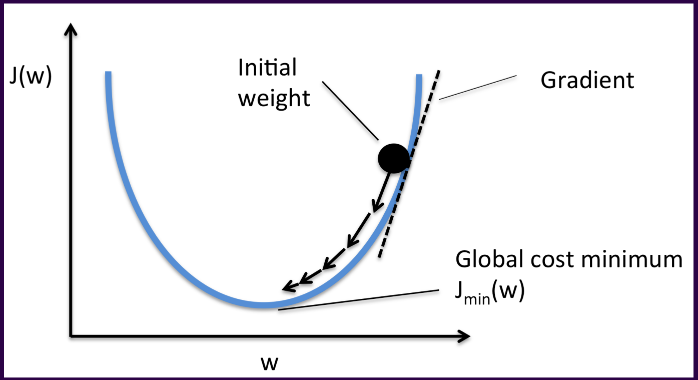
- Update Rule

  *Repeat*{

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

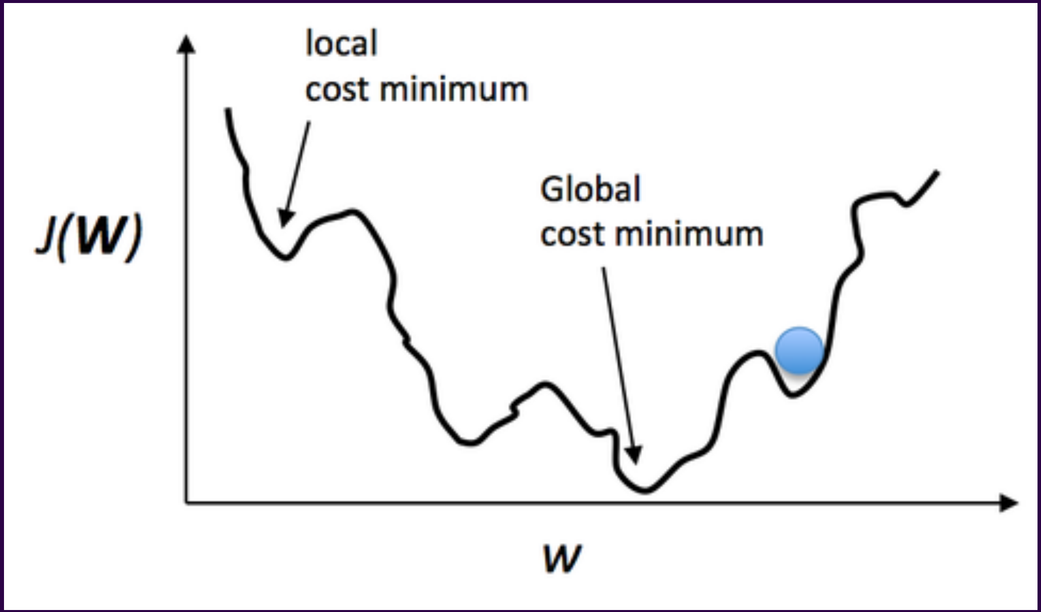
  }

  $\alpha$ is the learning rate

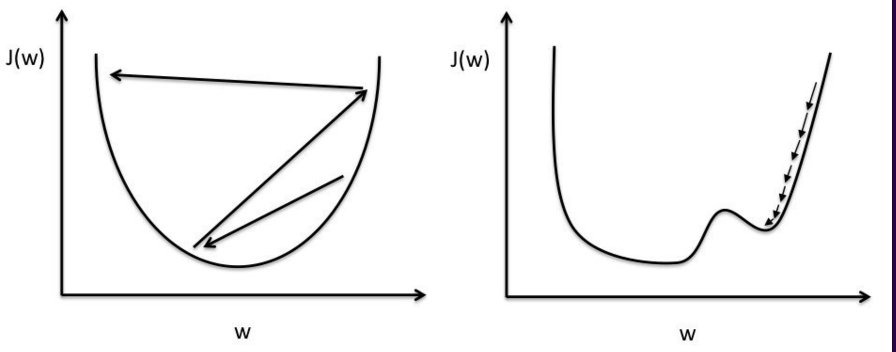


# General Loss Function Contours

- Most loss function contours are not perfectly parabolic
- Our goal is to find a solution that is very close to global minimum by the right choice of hyper-parameters

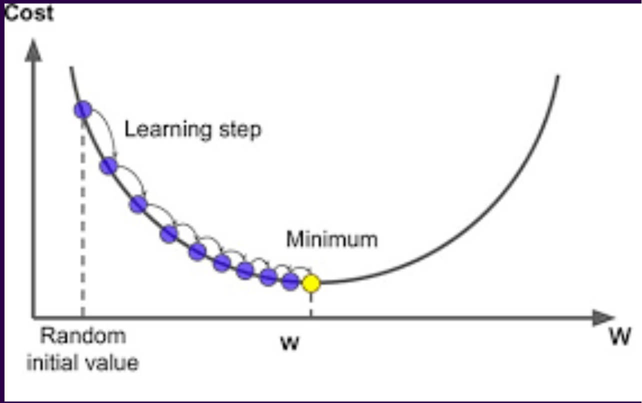


# Understanding Learning Rate




Large learning rate: Overshooting.

Small learning rate: Many iterations until convergence and trapping in local minima.




Correct learning rate

## Some Animations

- Demonstrate gradient descent animation

# Importance of Feature Normalization (Optional)

- Helps improve the performance of gradient based optimization