Day 3: Overfitting and Generalization

Summer STEM: Machine Learning

Department of Electrical and Computer Engineering
NYU Tandon School of Engineering
Brooklyn, New York

June 23, 2022

Outline

1. Review of Day 2
2. Polynomial Fitting
3. Regularization
4. Non-linear Optimization

NYU TANDON SCHOOL OF ENGINEERING

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)

Outline

1 Review of Day 2

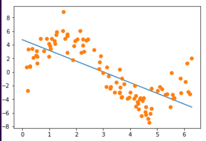
2 Polynomial Fitting

3 Regularization

4 Non-linear Optimization

Polynomial Fitting

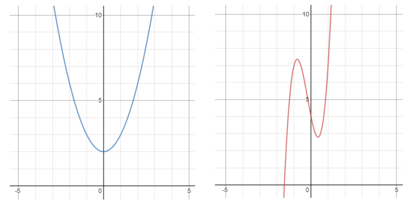
- We have been using straight lines to fit our data. But it doesn't work well every time
- Some data have more complex relation that cannot be fitted well using a straight line



- 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: $y = x^2 + 2$, $y = 5x^3 - 3x^2 + 4$



NYU TANDON SCHOOL OF ENGINEERING

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

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_N \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^M \\ 1 & x_2 & x_2^2 & \cdots & x_2^M \\ \vdots & & \ddots & & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^M \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_M \end{bmatrix}$$

- This can still be written as

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

- 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

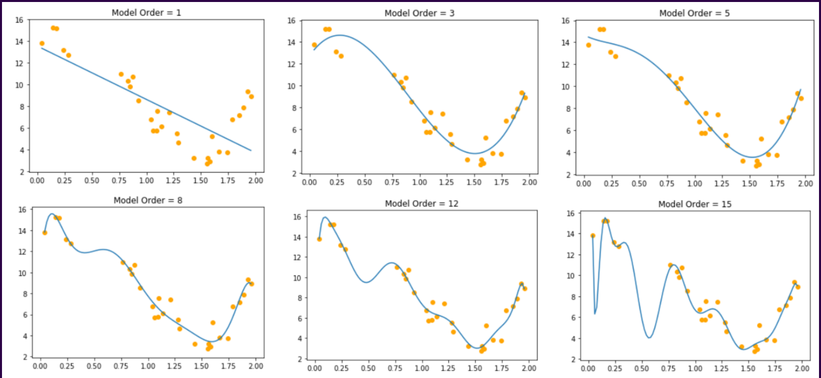
- Model $\hat{y} = \mathbf{w}^T \phi(\mathbf{x})$
- Loss $J(\mathbf{w}) = \frac{1}{N} \|Y - X\mathbf{w}\|^2$
- Find $\mathbf{w}$ that minimizes $J(\mathbf{w})$

NYU TANDON SCHOOL OF ENGINEERING

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



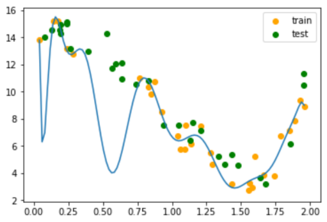
- Which of these model do you think is the best? Why?

Demo

Open demo_fit_polynomial.ipynb

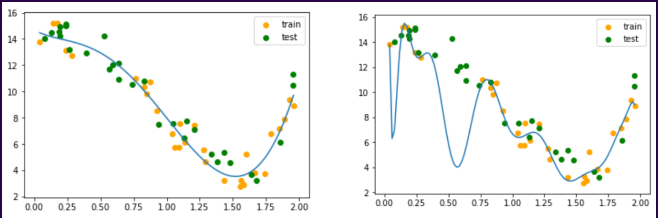
Overfitting

- 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

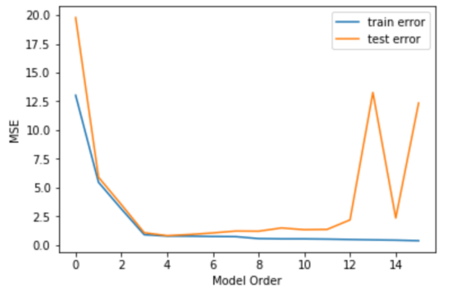
- Split the data set into a train set and a test set
- Train set will be used to train the model
- The test set will not be seen by the model during the training process
- Use test set to evaluate the model when a model is trained



- 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

1 Review of Day 2

2 Polynomial Fitting

3 Regularization

4 Non-linear Optimization

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

- **Regularization**: methods to prevent overfitting

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

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?

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?
  - Solution: We can change our cost function.

Weight Based Regularization

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

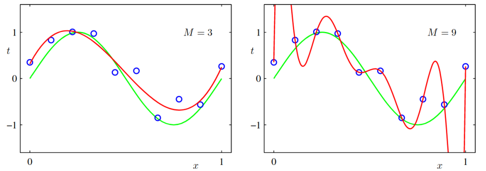


Table 1.1 Table of the coefficients $\mathbf{w}^{\star}$ for polynomials of various order. Observe how the typical magnitude of the coefficients increases dramatically as the order of the polynomial increases.

	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^{\star}$	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 λ a **hyper-parameter**
  - λ determines relative importance

Table 1.2 Table of the coefficients $\mathbf{w}^\star$ for $M = 9$ polynomials with various values for the regularization parameter λ. 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 λ 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

NYU TANDON SCHOOL OF ENGINEERING

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: λ 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 (λ)
  - **Test set**: to compute the performance of the algorithm (MSE)

Demo

Open demo_overfitting_regularization.ipynb

Outline

1 Review of Day 2

2 Polynomial Fitting

3 Regularization

4 Non-linear Optimization

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

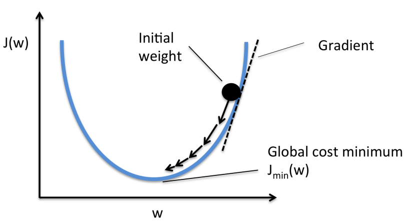
- Update Rule

  Repeat{

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

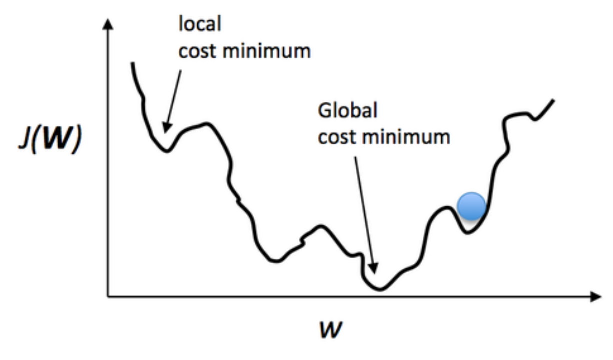
  }

  α is the learning rate

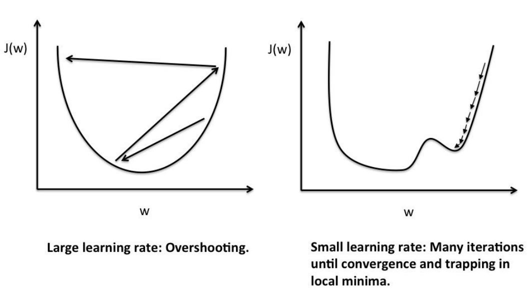


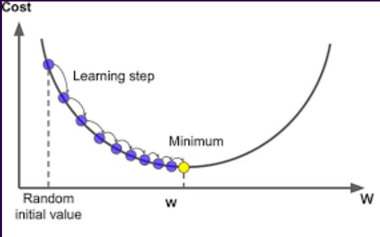
General Loss Function Contours

- 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





Correct learning rate

Some Animations

- Demonstrate gradient descent animation