Overfitting and Generalization

NYU K12 STEM Education: Machine Learning

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Course Details

- Course Website
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Outline

1. Review
2. Polynomial Fitting
3. Regularization
4. Optimization

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’

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
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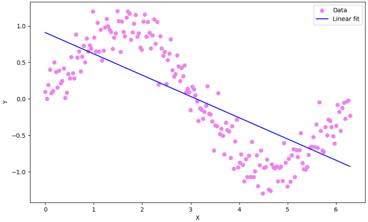
3. Regularization
4. Optimization

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



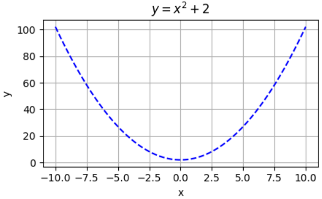
- Can we use some other model to fit this data?

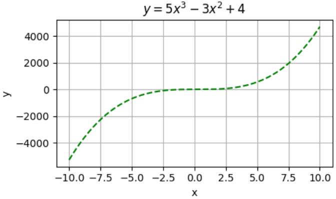
Polynomial Fitting

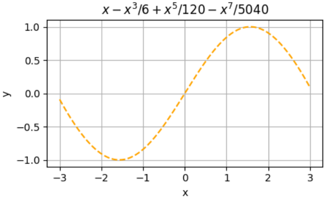
Can we use a polynomial to fit our data?

Polynomial: A sum of different powers of a variable

Example:







Polynomial Fitting

Polynomials of x: $\hat{y} = w_0 + w_1 x + w_2 x^2 + \cdots + w_m x^m$

m is called the order of the polynomial.

The process of fitting a polynomial is similar to linearly fitting multivariable data.

Polynomial Fitting

In matrix-vector form:

$$\begin{bmatrix} \hat{y_1} \\ \hat{y_2} \\ \vdots \\ \hat{y_N} \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^m \\ 1 & x_2 & x_2^2 & \cdots & x_2^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^m \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_m \end{bmatrix}$$

This can still be written as: $\hat{Y} = XW$

Loss:

$$J(W) = \frac{1}{N} ||Y - XW||^2$$

Polynomial Fitting

The i^{th} row of the design matrix X is simply a transformed feature:

$$\phi(x_i) = (1, x_i, x_i^2, \cdots, x_i^m)$$

Original Design Matrix:

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix}$$

Polynomial Fitting

Design matrix after feature transformation:

$$\begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^m \\ 1 & x_2 & x_2^2 & \cdots & x_2^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^m \end{bmatrix}$$

For the polynomial fitting, we just added columns of features that are powers of the original feature.

Linear Regression

Model:

$$\hat{y} = W^T \phi(x)$$

Loss:

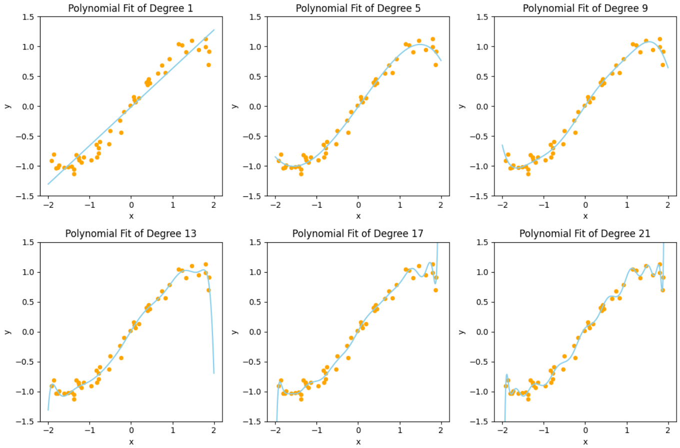
$$J(W) = \frac{1}{N} ||Y - XW||^2$$

Find W that minimizes $J(W)$

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



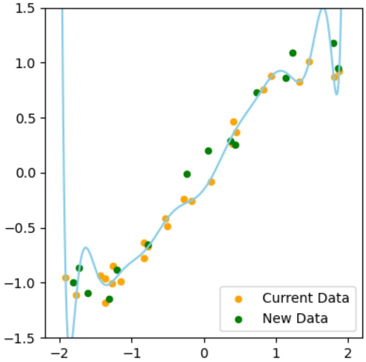
Which of these model do you think is the best? Why?

Overfitting

- Open Fit a Polynomial Demo

Overfitting

- 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 overfitting

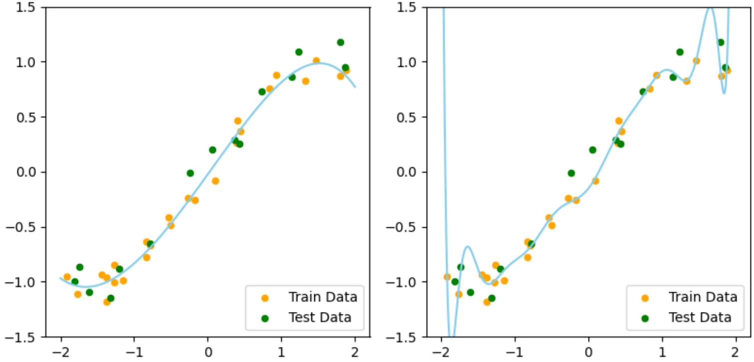


Solution to Overfitting

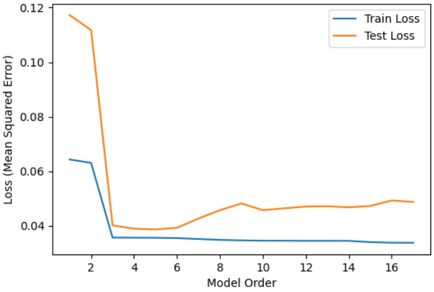
- Split the data set into a train set and a test set
- Train set will be used to train the model
- The test set will not be seen by the model during the training process
- Use test set to evaluate the model when a model is trained

Solution to Overfitting

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



Train and Test Loss



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

Outline

Regularization

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

- **Regularization:** methods to prevent overfitting
- One way to regularize is by model order selection.
- Is there another way?

Regularization

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

- **Regularization:** methods to prevent overfitting
- One way to regularize is by model order selection.
- Is there another way?
- We can change the cost function

Weight Based Regularization

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

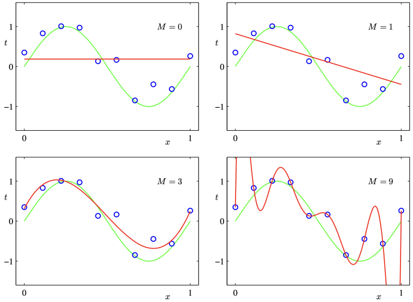


Table of the coefficients $\mathbf{w}^\star$ for polynomials of various order. Observe how the typical magnitude of the coefficients increases dramatically as the order of the polynomial increases.

	$M=0$	$M=1$	$M=6$	$M=9$
$w_0^\star$	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

Weight Based Regularization

New Cost Function:

$$J(W) = \frac{1}{N}||Y - XW||^2 + \lambda||W||^2$$

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

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

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.
  Example: λ weight regularization value vs. model weights (W)
- Solution: Split dataset into three:
  - **Training Set:** to compute the model parameters (W)
  - **Validation Set:** to tune the hyper-parameters (λ)
  - **Testing Set:** to compute the performance of the ML algorithm (MSE)

Overfitting and Regularization

- Open Overfitting, Weight Regularization Demo

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Non-linear Optimization

- 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

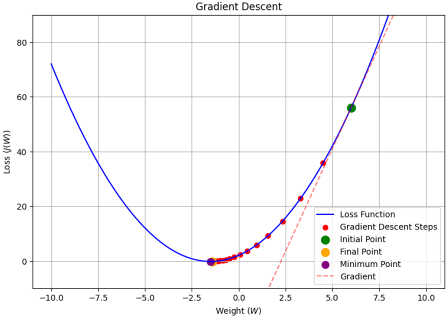
Update Rule:

Repeat{

$$W_{\text{new}} = W - \alpha \nabla J(W)$$

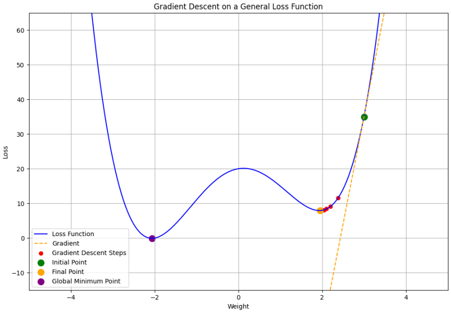
}

α is the learning rate

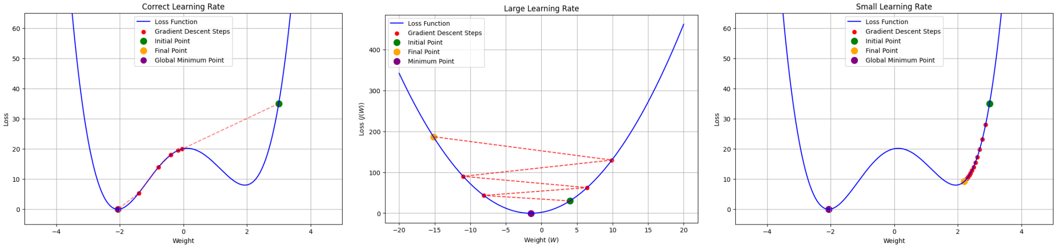


Loss Function Contours

- 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



Gradient Descent Animations