Regularization and Model Tuning

Week 5

Mo Esmalifalak, PhD

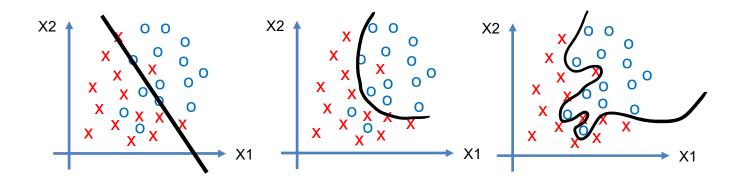


Model fitting issues

- One of the goals of machine learning is generalizability.
- If your model works only on your training data, the model is effectively useless.
- Depending on the training process your model might be
 - Underfitted
 - Overfitted
 - Well fitted



Over Fitting vs Under Fitting



Model performs well on the training data but generalizes poorly on test



Over fitting

Model performs poorly on both training and test



Under fitting

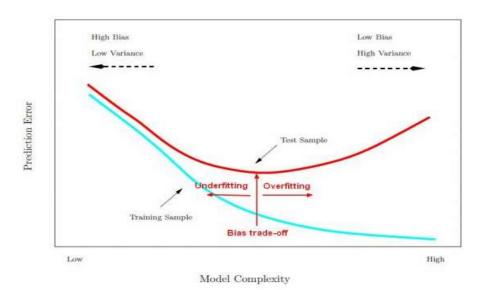
Overfitting vs Underfitting

Over-fitting

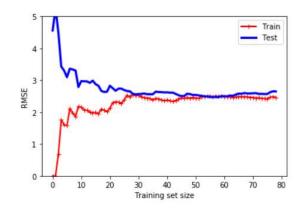
- · Generally occurs when a model is excessively complex.
- Sensitive to noise and other parameters which were not modeled during the training.

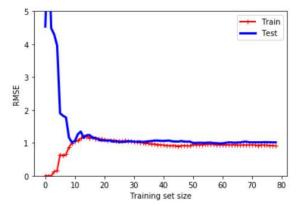
Under-fitting

- · Occurs when a model is over simplified
- · Number of training samples are not enough



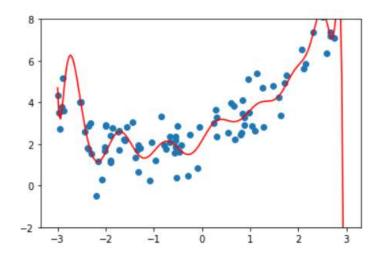
Over Fitting vs Under Fitting

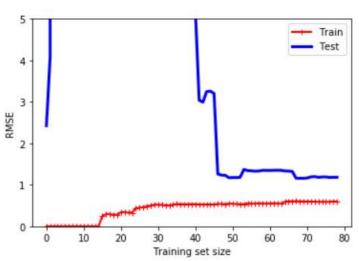




- 1- Low training RMSE and high testing RMS at beginning
- 2- Training data goes up until it reaches a **plateau**
- 3- Both curves have reached a plateau; they are close and fairly high (sign of under-fitting).
- 4- If model is under-fitting, adding more training data will not help.
 - 1- Low training RMSE and high testing RMS at beginning
 - 2- Training data goes up until it reaches a **plateau**
 - 3- Both curves have reached a plateau; they are close and fairly low (sign of fitting right).

Over Fitting vs Under Fitting





Higher complexity = better fit to training data (But less generalizable)

Low training RMSE but high testing RMS at steady state (sign of over-fitting).

One way to improve an overfitting model is to feed it more training data until the validation error reaches the training error.

How to avoid overfitting?

- Have a very large training data
- Reduce model complexity
- Regularization

Regularization (in General)

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

penalty='l2'
$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{i=1}^{n} \theta_i^2$$

penalty='I1'
$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{i=1}^{n} |\theta_i|$$

L2 regularization	L1 regularization
Computational efficient due to having analytical solutions	Computational inefficient on non-sparse cases
Non-sparse outputs	Sparse outputs
No feature selection	Built-in feature selection

Regularization (in linear regression)

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_{\theta} (x^{(i)}) - y^{(i)} \right)^{2}$$

Ridge Regression

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_{\theta} (x^{(i)}) - y^{(i)} \right)^2 + \frac{\alpha}{2} \sum_{i=1}^{n} \theta_i^2$$

Lasso Regression

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_{\theta} (x^{(i)}) - y^{(i)} \right)^2 + \alpha \sum_{i=1}^{n} |\theta_i|$$

Elastic Net
$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_{\theta} (x^{(i)}) - y^{(i)} \right)^2 + r\alpha \sum_{i=1}^{n} |\theta_i| + \frac{(1-r)\alpha}{2} \sum_{i=1}^{n} \theta_i^2$$

Gradient Descent

No Regularization:

Repeat, {
$$\theta_k := \theta_k - \frac{\alpha}{m} \sum_{i=1}^m (h_\theta \big(x^{(i)} \big) - y^{(i)}) x_k^{(i)}$$
 }

With Regularization:

```
Repeat, { \theta_k := \theta_k (\mathbf{1} - \alpha \frac{\lambda}{m}) - \frac{\alpha}{m} \sum_{i=1}^m (h_\theta \big( x^{(i)} \big) - y^{(i)}) x_k^{(i)} }
```

Linear Regression

No Regularization:

$$\theta = (X^T X)^{-1} X^T y$$

With Regularization:

(Ridge Regression)

$$\theta = (X^T X + \lambda \begin{bmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix})^{-1} X^T y$$

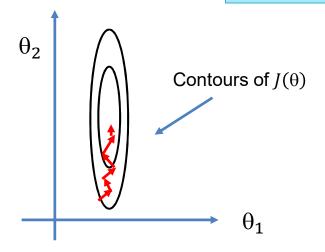
Feature Normalization

x1 = size of house: (1000-3000)

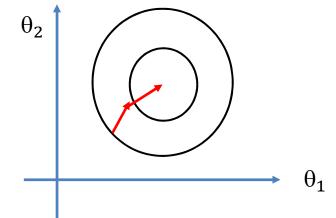
x2= # of bedrooms: (0-5)

x1= (x1-mean)/range: [-0.5,0.5] x2= # (x1-mean)/range: [-0.5,0.5]

$$\theta^T X = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$



Converging to global minimum is harder



Converging to global minimum is easier



© All rights reserved. All content within our courses, such as this video, is protected by copyright and is owned by the course author or unless otherwise stated. Third party copyrighted materials (for example, images and text) have either been licensed for use in any given course, or have been copied under an exception or limitation in Canadian Copyright law. For further information, please contact the McMaster University Centre for Continuing Education ccecrsdv@mcmaster.ca.