An Unknown Signal Report

George Herbert cj19328@bristol.ac.uk

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Abstract

This report demonstrates my understanding of the methods I have used, the results results I have obtained and my understanding of issues such as overfitting for the 'An Unknown Signal' coursework.

1 Equations for linear regression

For a set of points that lie along a line with Gaussian noise $\mathbf{y} = \mathbf{X}\mathbf{w} + \epsilon$ where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, the maximum likelihood esimation is equivalent to the least square error estimation and is given by the equation:

$$\hat{\mathbf{w}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}.$$

I've implemented this equation in my code as the following function:

def regressionNormalEquation(self, X, y):
return np.linalg.inv(X.T @ X) @ X.T @ y

- 2 Choice of polynomial order
- 3 Choice of unknown function

4 Overfitting

Overfitting occurs when a machine learning algorithm produces a model that has learnt the noise in the data as if it represents the structure of the underlying model. [1]

In the case of linear regression, overfitting is most likely to occur by producing a model with too complex a function type, such that it would fail to predict future observations.

5 Model selection

To prevent overfitting, I have used leave-one-out cross-validation when producing a model for each 20-point line segment. Leave-one-out cross-validation is an extreme case of k-fold cross validation such that k = n, where n is the number

of data-points (in this case 20). Despite being computationally expensive, I believe that leave-one-out cross-validation is an appropriate technique to prevent overfitting, due to the limited sample size of each line segment.

Leave-one-out cross-validation involves using each of the 20 data-points exactly once as validation data for a model trained using the other 19 data-points. The cross-validation error for each function type is calculated as follows [2]:

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}^{(-i)})^2$$

where n is the number of datapoints in a line segment (i.e. 20); y_i is the actual y-value for the i-th datapoint; and $\hat{y}^{(-i)}$ is the predicted y-value for the i-th datapoint, when trained without using the i-th sample.

The function type with the lowest cross-validation error is then selected.

6 Testing

7 Optimisations and improvements

- 1. Using np.linalg.solve
- 2. Not shuffling the data before leave-one-out cross-validation
- 3. Not finding the average cross-validation error
- 4. Using the linear regression leave-one-out shortcut

References

- [1] Burnham, K. P. and Anderson, D. R. (2002) Model Selection and Multimodel Inference. 2nd ed. Springer-Verlag.
- [2] Taylor, J. (2020) Leave one out cross-validation (LOOCV) https://web.stanford.edu/class/stats202/notes/Resampling/LOOCV.html