An Unknown Signal Report

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Abstract

This report demonstrates my understanding of the methods I have used, the 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 (x, y) coordinates that lie along a line with Gaussian noise, with the relationship $\mathbf{y} = \mathbf{X}\mathbf{w} + \epsilon$ where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, the maximum likelihood estimation of $\mathbf{w}$ is equivalent to the least square error estimation and is given by the equation:

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

This equation is implemented in my code as the following method:

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

$\mathbf{X}$ can take one of the following three forms:

$$\mathbf{X} = \begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_{20} & 1 \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} x_1^n & x_1^{n-1} & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ x_{20}^n & x_{20}^{n-1} & \dots & 1 \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} f(x_1) & 1 \\ \vdots & \vdots \\ f(x_{20}) & 1 \end{bmatrix}$$

depending on whether the line is linear, polynomial of degree n, or the unknown function f, respectively.

2 Choice of polynomial degree

Having created a program, '`display.py`', to visualise the points, I drew up a list of segments that appeared nonlinear. Then, I created a program, '`degree.py`', that calculated the cross-validation error for these line segments when trained using a model with a polynomial of degree 2 to a polynomial of degree 10; Table 1 shows a small section from the output of this program.

Having analysed the output, it was clear that a large proportion of the nonlinear signals had their minimum cross-validation error when fitted with a polynomial of degree 3. This

Table 1: Section of the output from '`degree.py`'

Filename	Line segment	Polynomial degree	Cross-validation error
basic_3.csv	0	2	7.3947610358752875
basic_3.csv	0	3	1.2989585613760917e-23
⋮	⋮	⋮	⋮
adv_3.csv	5	9	318.8443359827487
adv_3.csv	5	10	279.2750683133305

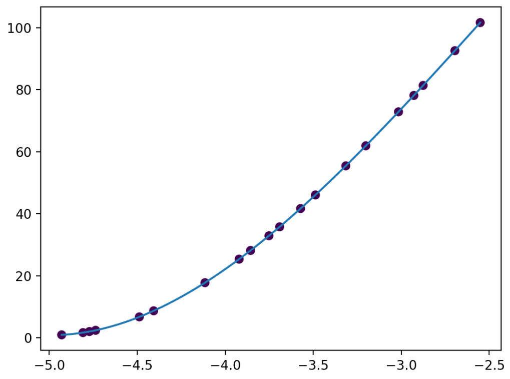


Figure 1: Plot for '`basic_3.csv`'

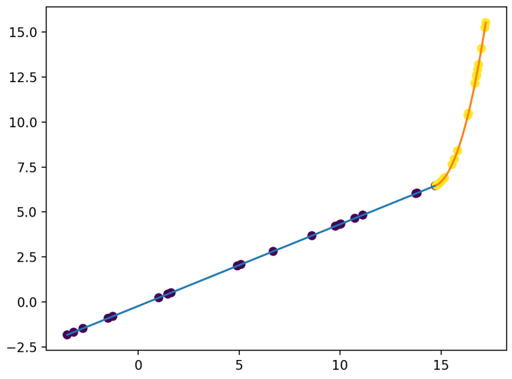


Figure 2: Plot for '`basic_4.csv`'

consistent minimum cross-validation error indicated that the polynomial line segments in the unknown signal are cubic.

Having incorporated cubic regression into my '`lsr.py`' least-squares regression program, I ran the program on the '`basic_3.csv`' and '`basic_4.csv`' unknown signals; Figure 1 and Figure 2 display these plots, respectively. The lines being a near-perfect fit allowed me to validate that a cubic polynomial is reasonable visually.

3 Choice of unknown function

Using my '`display.py`' program to visualise the signals, I produced a list of potential 'unknown functions' that could represent the underlying signal of line segments, based on their shapes: $\mathbf{w}_1 sin(x) + \mathbf{w}_2$, $\mathbf{w}_1 cos(x) + \mathbf{w}_2$, $\mathbf{w}_1 tan(x) + \mathbf{w}_2$ and $\mathbf{w}_1 e^x + \mathbf{w}_2$.

I then created a program, '`unknown.py`', that calculated the cross-validation error for each of the nonlinear line segments previously identified when trained using each of the potential unknown functions. A table displayed the cross-validation errors—similar to that used to determine the polynomial degree.

Having analysed the cross-validation errors, it was clear that all nonlinear signals that were likely not a cubic polynomial had their minimum cross-validation error when trained to fit the function $\mathbf{w}_1 sin(x) + \mathbf{w}_2$.

Having incorporated regression to fit a function of the form $\mathbf{w}_1 sin(x) + \mathbf{w}_2$ into my '`lsr.py`' least-squares regression program, I ran the program on the '`basic_5.csv`' and '`adv_3.csv`' unknown signals; the outputs are shown in Figure 3 and Figure 4 respectively. The lines being a near-perfect fit allowed me to validate that the unknown function is of

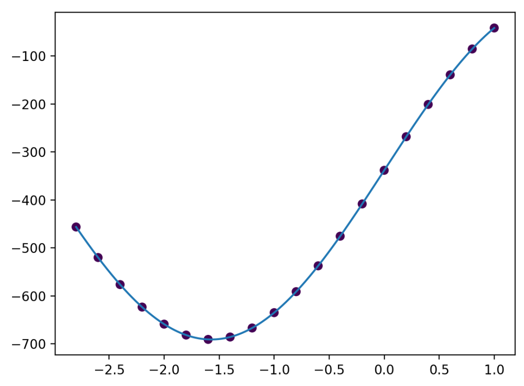


Figure 3: Plot for '`basic_5.csv`'

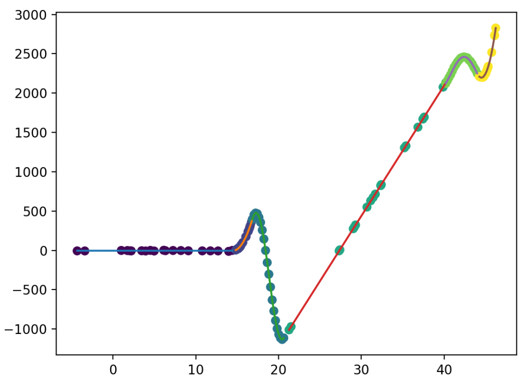
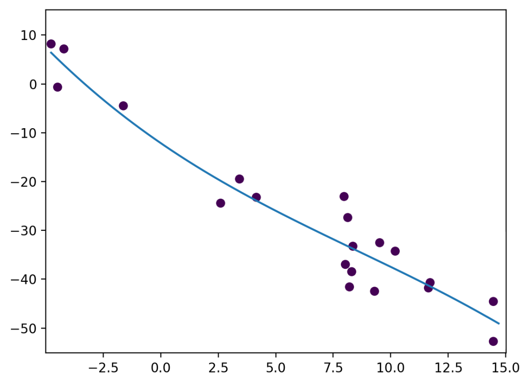


Figure 4: Plot for '`adv_3.csv`'

the form $\mathbf{w}_1 sin(x) + \mathbf{w}_2$ visually.

4 Model selection


(a) Cubic fit

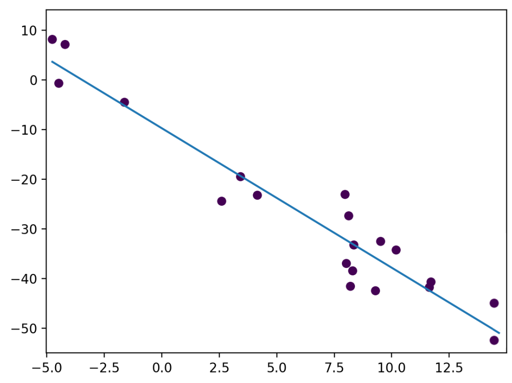

(b) Linear fit

Figure 5: Two fits for the first line segment in '`noise_2.csv`'

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. Figure 5 shows an example of this. On the left, (a) is a cubic fit that is too complex a function type for the data points. It would not predict future y-values for a set of given x-values as successfully as the linear fit (b) on the right.

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 in this case, owing 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 data points in a line segment (i.e. 20), y_i is the actual y-value for the i-th data point, and $\hat{y}^{(-i)}$ is the predicted y-value for the i-th data point when trained without using the i-th sample.

The function type with the lowest cross-validation error is then selected for each line segment, and the weights $\hat{\mathbf{w}}$ are determined by training on all data points for that segment.

5 Optimisations and improvements

To begin with, computing the matrix inverse using the `np.linalg.inv` method is computationally expensive and unnecessary. Instead, given $\mathbf{X}$ and $\mathbf{y}$, the maximum likelihood estimation of $\mathbf{w}$ could be directly computed as follows: `np.linalg.solve(X.T @ X, X.T @ y)`. Computing $\hat{\mathbf{w}}$ directly would be faster, as `np.linalg.inv` computes the inverse of a matrix $\mathbf{A}$ by solving for $\mathbf{A}^{-1}$ in $\mathbf{A}\mathbf{A}^{\mathbf{-1}} = \mathbf{I}$ [3]. Thus, there would be a performance benefit by solving for $\hat{\mathbf{w}}$ in $\mathbf{X}^T\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}^T\mathbf{y}$ directly.

Another computationally expensive operation in my algorithm is that used to calculate the cross-validation error using leave-one-out cross-validation. The method currently involves fitting the model and calculating the sum squared error n times. Instead, there exists a faster method I could have adopted that involves calculating the leverage. Despite this, I opted not to include this method because my program, as it currently stands, can be easily adapted to use k-fold cross-validation for any value of k that is a factor of 20—changing the constant '`K`' in the code achieves this.

6 Testing

I created a file, '`test.py`', that uses the `unittest` framework to test each of the methods in '`lsr.py`'.

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) — STATS 202* https://web.stanford.edu/class/stats202/notes/Resampling/LOOCV.html

[3] Muldal, A. (2017) *Why does numpy.linalg.solve() offer more precise matrix inversions than numpy.linalg.inv()?* https://stackoverflow.com/a/31257909/8540479