An Unknown Signal Report

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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

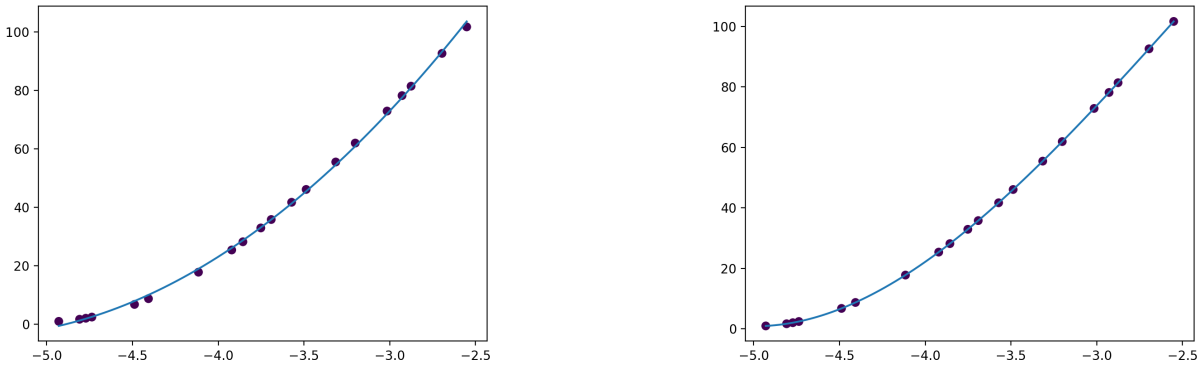
I used several different techniques to determine and validate that the polynomial degree used to genereate the unknown signals was likely cubic.

Firsly, a polynomial of degree n can have a maximum of $n-1$ relative extrema. Across all of the unknown signals, no line segment appeared to have more than two relative extrema. This made it is likely, but not definitive, that the polynomial degree was relatively low (e.g. cubic, quartic). However, there was still a possibility the polynomials used to generate the unknown signals were of a higher degree, and that the segments chosen just happened to display the characteristics of a lower-degree polynomial (e.g. low number of relative extrema).

To better identify exactly which polynomial degree was used to generate the unknown signals, I created a program '`display.py`' to visualise the points. By inspecting the appearance of each segement, I drew up a list of nonlinear segments. I then 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

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



(a) Quadratic fit

(b) Cubic fit

Figure 1: Two fits for '`basic_3.csv`'

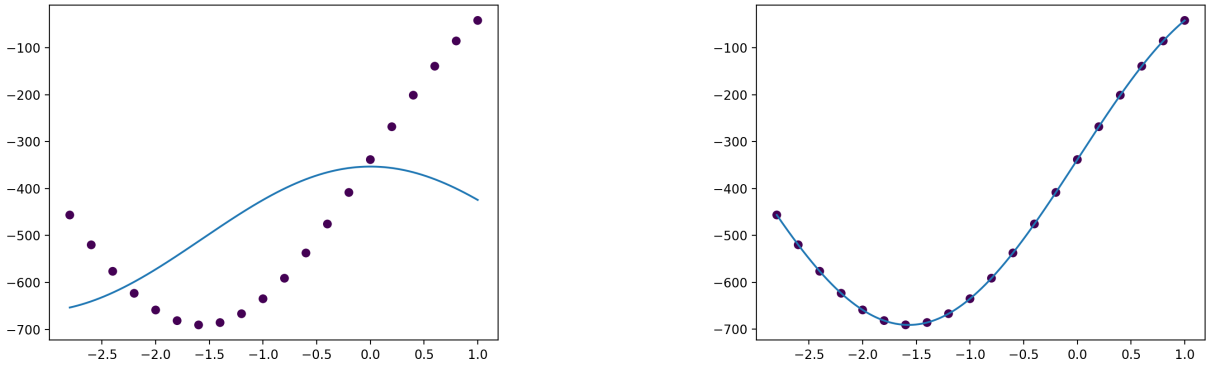
of degree 3. This consistent minimum cross-validation error indicated that the polynomial line segments in the unknown signal are cubic.

To confirm this visually, I used the '`basic_*.csv`' files as they have a negligable amount of noise. I produced fits using several different polynomials. An example of this is shown in Figure 1. The quadratic fit shown in Figure 1a is clearly not as good a fit as the cubic fit shown in Figure 1b.

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 $\mathbf{w}_1 sin(x) + \mathbf{w}_2$. This consistent minimum cross-validation error indicated that the 'unknown function' used to generate the unknown signals is of the form $\mathbf{w}_1 sin(x) + \mathbf{w}_2$.

'`basic_5.csv`' was the only one of the '`basic_*.csv`' files to not fit linear and cubic functions exactly, which strongly indicated that it was generated from the unknown function. Thus, due to its negligable amount of noise, I used it to verify that the unknown function was $\mathbf{w}_1 sin(x) + \mathbf{w}_2$. To do so, I produced a fit for each of the potential unknown functions. An example of this is



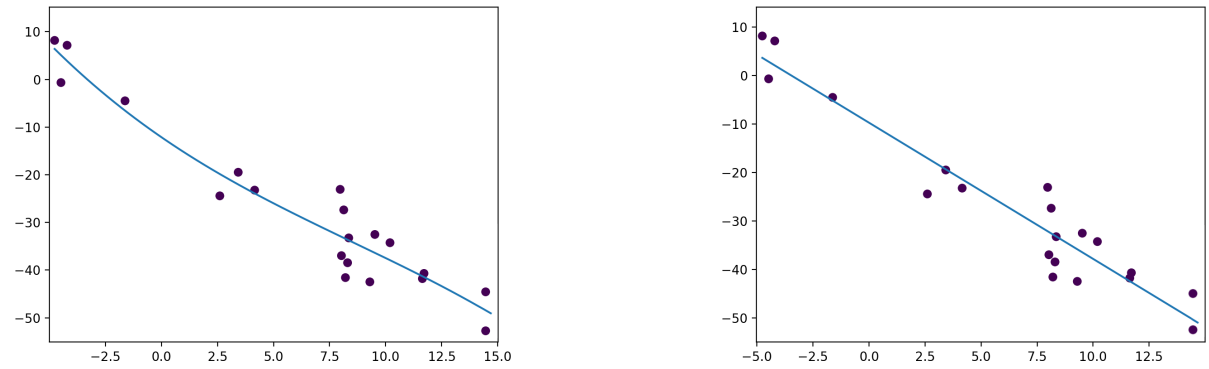
(a) Cosine fit

(b) Sine fit

Figure 2: Two fits for '`basic_3.csv`'

shown in Figure 2. The cosine fit shown in Figure 2a is a far worse fit than the sine fit shown in Figure 2b, which fits almost perfectly.

4 Model selection



(a) Cubic fit

(b) Linear fit

Figure 3: 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 3 shows an example of this. Figure 3a shows 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 shown in Figure 3b

My original implementation used the holdout method to detect overfitting, and determine the best model for a given line segment. However, despite experimenting with different sized training and validation sets, my program was consistently giving misleading results—both overfitting and underfitting. This is because the holdout method involved only a single run, and so was dependent on how the datapoints were randomly split into training and validation sets.

Due to the limited number of data points in each line segment, this resulted in the program often providing wildly different results. On the other hand, as the holdout method only involved a single run, it was fast.

Despite the speed of the holdout method, I wanted my increase the accuracy of my program. To do so, I implemented k-fold cross-validation. In particular, I opted to use 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). As a result of having to produce n different models, leave-one-out cross-validation can be computationally expensive. However, owing to the limited sample size of each line segment, I believe it to be an appropriate technique in this case.

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 $\mathbf{AA^{-1}} = \mathbf{I}$ [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