Linear Regression, Method 1

Chris Cornwell

Feb 11, 2025

Outline

Overview of linear regression task

The procedure

Implementing the procedure

Examples

Outline

Overview of linear regression task

The procedure

Implementing the procedure

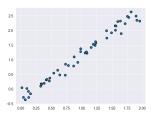
Examples

The goal

- Setting: have points in the plane, say n of them. Say the points are $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$.
- Goal: Model them as being "noisy" points from a line, finding "best fit" line (the closest linear model). This line is also called the least squares regression (LSR) line.

The goal

- Setting: have points in the plane, say n of them. Say the points are $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$.
- Goal: Model them as being "noisy" points from a line, finding "best fit" line (the closest linear model). This line is also called the least squares regression (LSR) line.
- Running example: A data set, 'Example1.csv', with 50 points, is available here; these points are displayed in the plot.



Outline

Overview of linear regression task

The procedure

Implementing the procedure

Examples

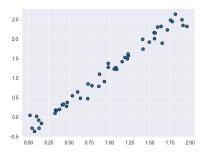


Figure: Our running example

How do we find the LSR line?

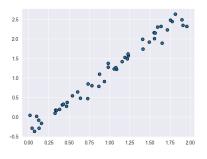


Figure: Our running example

How do we find the LSR line?

Can get the slope m, intercept b simply from using the polyfit function in NumPy. If x, y are the arrays with x- and y-coordinates:

```
np.polyfit(x,y,1)
```

But, how are the slope, intercept found?

 $^{^{1}}$ Will use \mathbf{p} for this vector, for the rest of these slides.

But, how are the slope, intercept found?

If a slope m and intercept b existed so that $(x_1, y_1), \ldots, (x_{50}, y_{50})$ were points on y = mx + b, then

$$y_i = mx_i + b$$

would hold for all $1 \le i \le 50$.

 $^{^{1}}$ Will use \mathbf{p} for this vector, for the rest of these slides.

But, how are the slope, intercept found?

If a slope m and intercept b existed so that $(x_1, y_1), \ldots, (x_{50}, y_{50})$ were points on y = mx + b, then

$$y_i = mx_i + b$$

would hold for all $1 \le i \le 50$.

1. Write those 50 equations as a matrix equation. Setting:

$$\mathbf{A} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_{50} & 1 \end{bmatrix}; \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{50} \end{bmatrix},$$

and writing¹ $\mathbf{p} = \begin{bmatrix} m \\ b \end{bmatrix}$, the matrix equation is $A\mathbf{p} = \mathbf{y}$.

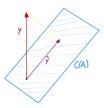
 $^{^{1}}$ Will use \mathbf{p} for this vector, for the rest of these slides.

Now the equation $A\mathbf{p} = \mathbf{y}$ does not have a solution (those points are *not* on a line).

Now the equation $A\mathbf{p} = \mathbf{y}$ does not have a solution (those points are *not* on a line).

Next idea: (thinking of noise being in y-coordinate direction)

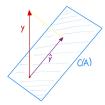
• Get vector $\hat{\mathbf{y}}$ that is as close to \mathbf{y} as possible, so that $A\mathbf{p} = \hat{\mathbf{y}}$ has a solution.



Now the equation $A\mathbf{p} = \mathbf{y}$ does not have a solution (those points are *not* on a line).

Next idea: (thinking of noise being in y-coordinate direction)

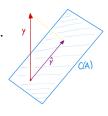
- Get vector $\hat{\mathbf{y}}$ that is as close to \mathbf{y} as possible, so that $A\mathbf{p} = \hat{\mathbf{y}}$ has a solution.
- For each *i*, we either increase or decrease y_i by a (hopefully small) amount, $y_i \rightsquigarrow \hat{y}_i$. We make $|\mathbf{y} \hat{\mathbf{y}}|$ as small as possible.



Now the equation $A\mathbf{p} = \mathbf{y}$ does not have a solution (those points are *not* on a line).

Next idea: (thinking of noise being in y-coordinate direction)

- ▶ Get vector $\hat{\mathbf{y}}$ that is as close to \mathbf{y} as possible, so that $A\mathbf{p} = \hat{\mathbf{y}}$ has a solution.
- For each *i*, we either increase or decrease y_i by a (hopefully small) amount, $y_i \rightsquigarrow \hat{y}_i$. We make $|\mathbf{y} \hat{\mathbf{y}}|$ as small as possible.
- 2. Done by solving $A^{T}A\mathbf{p} = A^{T}\mathbf{y} \text{ (normal equations)}.$ If $\mathbf{p} = \begin{bmatrix} \hat{m} \\ \hat{b} \end{bmatrix}$ is the solution, then $\hat{\mathbf{y}}$ is given by $A \begin{bmatrix} \hat{m} \\ \hat{b} \end{bmatrix}$.



Why does solving $A^TAp = A^Ty$ give the right thing?

Why does solving $A^T A \mathbf{p} = A^T \mathbf{y}$ give the right thing?

Related to orthogonal vectors in \mathbb{R}^n (in the example, \mathbb{R}^{50}).

If $A\mathbf{p} = \hat{\mathbf{y}}$ has a solution, then $\hat{\mathbf{y}} \in \mathbb{R}^{50}$ is in column space of A.

Why does solving $A^T A \mathbf{p} = A^T \mathbf{y}$ give the right thing?

Related to orthogonal vectors in \mathbb{R}^n (in the example, \mathbb{R}^{50}).

- If $\mathbf{A}\mathbf{p}=\hat{\mathbf{y}}$ has a solution, then $\hat{\mathbf{y}}\in\mathbb{R}^{50}$ is in column space of A.
- $\mathbf{y} = \mathbf{z}_1 + \mathbf{z}_2$, where \mathbf{z}_1 in null space of \mathbf{A}^T and \mathbf{z}_2 in column space of \mathbf{A} .

(Note: Null space of A^T orthogonal to column space of A.)

Why does solving $A^T A \mathbf{p} = A^T \mathbf{y}$ give the right thing?

Related to orthogonal vectors in \mathbb{R}^n (in the example, \mathbb{R}^{50}).

- If $\mathbf{A}\mathbf{p}=\hat{\mathbf{y}}$ has a solution, then $\hat{\mathbf{y}}\in\mathbb{R}^{50}$ is in column space of A.
- $\mathbf{y} = \mathbf{z}_1 + \mathbf{z}_2$, where \mathbf{z}_1 in null space of \mathbf{A}^T and \mathbf{z}_2 in column space of \mathbf{A} .
 - (Note: Null space of \mathbf{A}^T orthogonal to column space of \mathbf{A} .)
- lacktriangle As \mathbf{z}_2 in column space, $\exists~\hat{\mathbf{p}}$ so that $A\hat{\mathbf{p}}=\mathbf{z}_2$.

Why does solving $A^T A \mathbf{p} = A^T \mathbf{y}$ give the right thing?

Related to orthogonal vectors in \mathbb{R}^n (in the example, \mathbb{R}^{50}).

- If $A\mathbf{p} = \hat{\mathbf{y}}$ has a solution, then $\hat{\mathbf{y}} \in \mathbb{R}^{50}$ is in column space of A.
- $\mathbf{y} = \mathbf{z}_1 + \mathbf{z}_2$, where \mathbf{z}_1 in null space of \mathbf{A}^T and \mathbf{z}_2 in column space of \mathbf{A} .

(Note: Null space of A^T orthogonal to column space of A.)

lacktriangle As \mathbf{z}_2 in column space, $\exists~\hat{\mathbf{p}}$ so that $\mathsf{A}\hat{\mathbf{p}}=\mathbf{z}_2$. But then,

$$A^{\mathsf{T}}(A\hat{\mathbf{p}}) = A^{\mathsf{T}}\mathbf{z}_2 = A^{\mathsf{T}}(\mathbf{y} - \mathbf{z}_1) = A^{\mathsf{T}}\mathbf{y}.$$

And \mathbf{z}_2 is closest, since subtracted \mathbf{z}_1 from \mathbf{y} , orthogonal to column space:

$$\mathbf{z}_2 = \hat{\mathbf{y}}.$$

Normal equations:

$$(A^TA)\mathbf{p} = A^T\mathbf{y}.$$

Normal equations:

$$(A^TA)\mathbf{p} = A^T\mathbf{y}.$$

Note:

► A^TA is 2×2 matrix, $A^Ty \in \mathbb{R}^2$, and A^TA is invertible as long as there exists $x_i \neq x_i$.

Normal equations:

$$(A^TA)\mathbf{p} = A^T\mathbf{y}.$$

Note:

- ► A^TA is 2×2 matrix, $A^Ty \in \mathbb{R}^2$, and A^TA is invertible as long as there exists $x_i \neq x_i$.
- 3. Pretty straightforward to find solution to $(A^TA)\mathbf{p} = A^T\mathbf{y}$.

Normal equations:

$$(A^TA)\mathbf{p} = A^T\mathbf{y}.$$

Note:

- ► A^TA is 2×2 matrix, $A^Ty \in \mathbb{R}^2$, and A^TA is invertible as long as there exists $x_i \neq x_i$.
- 3. Pretty straightforward to find solution to $(A^TA)\mathbf{p} = A^T\mathbf{y}$.

So, three steps:

- 1. Write the *n* equations in matrix form. (get matrix A, vector y)
- 2. Get matrix A^TA and vector A^Ty for normal equations: $A^TAp = A^Ty$.
- 3. Use a method to solve normal equations for ${f p}$.

Outline

Overview of linear regression task

The procedure

Implementing the procedure

Examples

Solving normal equation, in pseudocode

Procedure to carry out the steps:

- 1. Write the *n* equations in matrix form. (get matrix A, vector y)
- 2. Get matrix A^TA and vector A^Ty for normal equations: $A^TAp = A^Ty$.
- 3. Use a method to solve normal equations for ${f p}$.

Solving normal equation, in pseudocode

Procedure to carry out the steps:

- 1. Write the n equations in matrix form. (get matrix A, vector y)
- 2. Get matrix A^TA and vector A^Ty for normal equations: $A^TAp = A^Ty$.
- 3. Use a method to solve normal equations for \mathbf{p} .

Given $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$, as a NumPy array (call it D, with shape (n, 2)):

```
\begin{array}{l} A \leftarrow \left[\text{x coordinates, all 1s}\right] \text{ \# 2-column matrix} \\ y \leftarrow y \text{ coordinates} \\ \text{\# next, get 2x2 matrix and 2-vector} \\ \text{Compute A.T times A; compute A.T times y} \\ \text{Solve normal eq'ns (numpy solve, or use inverse)} \\ \textbf{\textit{return}} \text{ solution} \end{array}
```

Outline

Overview of linear regression task

The procedure

Implementing the procedure

Examples

Result on running example

For the data (linked to above) with 50 points, the LSR line comes out close to

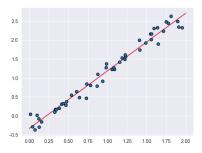
$$y = 1.520275x - 0.33458.$$

Result on running example

For the data (linked to above) with 50 points, the LSR line comes out close to

$$y = 1.520275x - 0.33458.$$

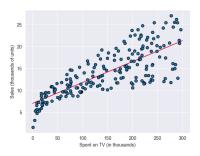
A plot of the line (in red), alongside the points, looks as follows.



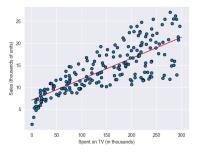
In the DataSets folder, the 'Advertising.csv' file contains data on amounts spent (in thousands of dollars) on TV, Radio, and Newspaper advertising in 200 different markets, as well as the amounts sold in each market (in thousands of units).

In the DataSets folder, the 'Advertising.csv' file contains data on amounts spent (in thousands of dollars) on TV, Radio, and Newspaper advertising in 200 different markets, as well as the amounts sold in each market (in thousands of units).

We will look more at this data later. For now, plotted here are the columns ('TV', 'Sales').

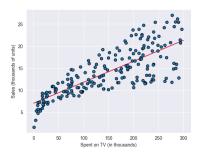


If you switch the role of x- and y-coordinates, you can still do linear regression; i.e., for purpose of a thought experiment, predict the TV data as the *response*, instead of the Sales.



If you switch the role of x- and y-coordinates, you can still do linear regression; i.e., for purpose of a thought experiment, predict the TV data as the *response*, instead of the Sales.

The LSR line for the data is then **not** the same line, if you switch the roles of TV and Sales in the algorithm to get $\hat{\mathbf{p}}$.



If you switch the role of x- and y-coordinates, you can still do linear regression; i.e., for purpose of a thought experiment, predict the TV data as the *response*, instead of the Sales.

The LSR line for the data is then **not** the same line, if you switch the roles of TV and Sales in the algorithm to get $\hat{\mathbf{p}}$.

