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< Previous



Next >

8. Summary

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Summarize

Big Picture

Given a set of data points, (x_i, y_i) the simplest possible relationship we can hope to find between the data is a linear one. That is, we want to find a line $y = ax + b$ that best fits these data. Our "variables" are now the a and b , the slope and y -intercept that determine the linear relationship.

In order to find the best possible a and b , we minimize an error function. The error function we defined squares the difference between the y_i to the predicted value $ax_i + b$:

$$D(a, b) = \sum_{i=1}^n (y_i - (ax_i + b))^2.$$

Thus finding the best fit requires minimizing this function of two variables a and b , which is an (unconstrained) optimization problem!

Mechanics

To fit a collection of data (x_i, y_i) to a straight line that minimizes the squares of the differences between the predicted y values and the actual y_i , solve the system:

$$\left(\sum_{i=1}^n x_i^2 \right) a + \left(\sum_{i=1}^n x_i \right) b = \sum_{i=1}^n x_i y_i \quad (4.218)$$

$$\left(\sum_{i=1}^n x_i \right) a + nb = \sum_{i=1}^n y_i. \quad (4.219)$$

where n is the number of data points.

- To fit your data (x_i, y_i) to a power law $y = cx^p$, first transform your data $(X_i, Y_i) = (\ln x_i, \ln y_i)$, then use least squares approximation. The power p will be the slope.
- To fit your data (x_i, y_i) to an exponential law $y = ce^{kx}$, first transform your data $(X_i, Y_i) = (x_i, \ln y_i)$. Then use least squares approximation. The exponential multiple k is the slope of the least squares fitting to the transformed data.

Ask Yourself

▼ Why is it called least-squares approximation?

In order to define "best fit" we have to make a decision about how to quantify the error. A common choice is to minimize the square of the difference between predicted and observed values. Since this method involves minimizing squares, the method is called "least-squares".

[Hide](#)

▼ What is the point of drawing a straight line through data?

Fitting a straight line to data isn't just for making pretty pictures! Once we have a line that fits our data well, we can "extrapolate", which means we can make a prediction for what would have happened for values we weren't able to test. For example, if you find the line of best-fit between x = heights of marathon runners and y = marathon time, then you can use the line to predict the time for a new marathon runner, even if all you know is their height. Of course the prediction won't be perfect, but it's a good start. If you study statistics, you can learn how to create a "confidence interval" around the predicted

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In this sense, least squares approximation is an example of **machine learning**, the process by which a computer can be "trained" on some data (here it would be the (x_i, y_i) pairs that we measure) and the computer "learns" to predict what would happen for other data (new values of x_i outside of the training set).

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8. Summary

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Topic: Unit 3: Optimization / 8. Summary

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< Previous

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11 min + 4 activities

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