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Theory:

To fit a curve to the given data set, we need to find a mathematical function/model which is as close as possible to the given data set. It means that the value of the function should be as close as possible to the observed value in the data set at every point in the graph.

Goodness of fit:

We can find many curves which could fit the given data to some degree. However, to find the best curve among them, there should be some way to measure the “goodness” of the fit for that curve.

One such measure is the R-square method. It's calculated as follows.

Let the function $y = f(x)$ be the curve that is used for fitting. Then, the error in each of the points with respect to this function would be as follows.

$$\text{Error} = |y(i) - \text{value of } f(x) \text{ at } x(i)| = |y(i) - f(x(i))|$$

Another quantity called sum of squared error is defined as follows.

$$SSE(\text{sum of squared errors}) = \sum_{i=1}^n \text{Error}(i)^2$$

The mean of the values of the function would be as follows.

$$\text{Mean} = \frac{1}{n} \sum_{i=1}^n f(x(i))$$

The sum of the square of the difference between the value of the function at a given point and the mean is termed as SSR(sum of squares of regression).

$$SSR = \sum_{i=1}^n (f(x(i)) - \text{Mean})^2$$

Then, the sum of square total(SST) is defined as follows.

$$SST = SSR(\text{Sum of squares of regression}) + SSE(\text{sum of squared error})$$

A quantity called R-square is used to measure how good the fit is in explaining the variation in the data. The square of the correlation between the response values and the predicted values is equal to the R-squared.

$$R^2 = SSR/SST$$