

Calculus for the Life Sciences I

Lecture Notes – Least Squares Analysis

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Outline

- 1 Least Squares Analysis
 - C Period for *E. coli*
 - Pulse Labeling Experiment
 - Linear Model for C Period
- 2 Least Squares Best Fit
 - Error between Line and Data
 - Least Square Formula
 - C Period Example
- 3 Worked Example 1
 - Juvenile Growth Model - Revisited
 - Two Research Models
- 4 Error Analysis
 - Percent and Relative Error
- 5 Worked Example 2
 - Growth Model

Linear Least Squares Best Fit

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- **Linear least squares best fits** a linear model to data

Linear Least Squares Best Fit

- Linear Models section showed cricket data appear to lie on a line
- **Linear least squares best fits** a linear model to data
- **Linear regression** is another common name for this analysis
 - The term regression comes from a pioneer in the field of applied statistics who gave the least squares line this name because his studies indicated that the stature of sons of tall parents reverts or regresses toward the mean stature of the population

Cell Division in *E. coli*

Figures for Cell Cycle for *E. coli*

- Genome is a single large loop of DNA (3,800,000 base pairs)
- Replicates in both directions, starting at *oriC*
- Bacteria (prokaryotes) cell cycle differs from eukaryotic organisms – replication cycles overlap for rapid growth

Cell Cycle in *E. coli*

Replication of DNA in *E. coli*

- *Escherichia coli* can divide every 20 minutes
- Time for the DNA to replicate is the **C period**
- Time for the two loops of DNA to split apart, segregate, and form two new daughter cells is the **D period**
- The **C period** is 35-50 min, and the **D period** is over 25 min
- Replication cycle often longer than cell division time
- Up to 8 *oriCs* in a single *E. coli*

Pulse Labeling Experiment

Finding the C Period

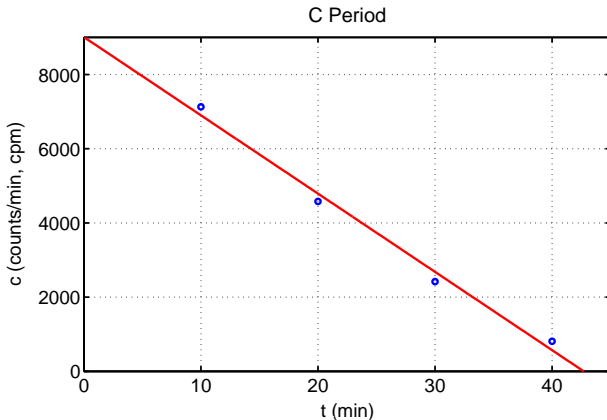
- A pulse of radioactive thymidine given to *E. coli*
- Drugs at $t = 0$ to stop new replication forks and division
- Radioactive thymidine added to existing forks
- As forks end, no new radioactive thymidine added
- Radioactive emissions, c in counts/min (cpm) measured in lab of Prof. Judith Zyskind (SDSU)

t (min)	10	20	30	40
c (cpm)	7130	4580	2420	810

Linear Model for C Period – Graph

Best fitting Linear Model for C Period

$$c = -211.2t + 9015$$



Fitting the Data

Linear Model

$$c = at + b$$

- Actual model uses techniques of Integral Calculus
- Linear model a reasonable approximation

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- Minimizes distance by adjusting slope, a , and intercept, b

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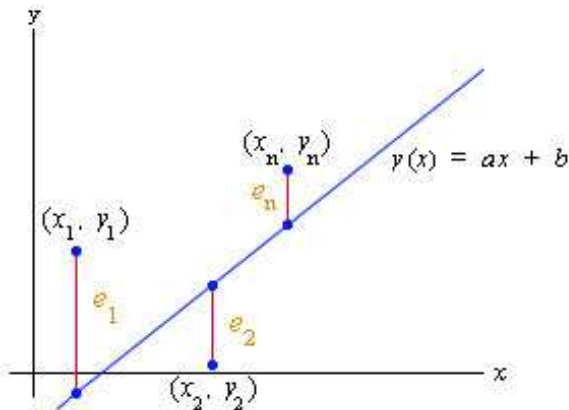
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- **Least squares best fit** minimizes sum of c -distance from data to linear model
- Minimizes distance by adjusting slope, a , and intercept, b

Data suggest that **C period** is 42.7 min

Least Squares Best Fit

The **least squares best fit** of a line to data is the best line through a set of data



Fitting the Data

- Consider a set of n data points:

$$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$$

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- The least squares best fit minimizes the square of the error in the distance between the y_i values of the data points and the y value of the line
- Distance depends on selection of the slope, a , and the intercept, b

Error between Line and Data

- Error between each of the data points and the line is

$$e_i = y_i - y(x_i) = y_i - (ax_i + b), \quad i = 1, \dots, n$$

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- The error e_i varies as a and b vary

Sum of Square Errors

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$$J(a, b) = e_1^2 + e_2^2 + \dots + e_n^2 = \sum_{i=1}^n e_i^2$$

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Minimum is determined using Calculus of two variables

Formula for Best Fitting Line

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The best fitting intercept satisfies

$$b = \frac{1}{n} \sum_{i=1}^n y_i - a\bar{x} = \bar{y} - a\bar{x}$$

C Period Example (continued)

The **pulse labeling** experiment for *E. coli* gave data points:

$$(10, 7130), (20, 4580), (30, 2420), (40, 810)$$

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The mean time is

$$\bar{t} = \frac{10 + 20 + 30 + 40}{4} = 25$$

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$$(10, 7130), (20, 4580), (30, 2420), (40, 810)$$

The mean time is

$$\bar{t} = \frac{10 + 20 + 30 + 40}{4} = 25$$

The best slope, a , satisfies

$$a = \frac{(10-25)7130 + (20-25)4580 + (30-25)2420 + (40-25)810}{(10-25)^2 + (20-25)^2 + (30-25)^2 + (40-25)^2}$$
$$a = -211.2$$

C Period Example (continued)

Similarly, the c -intercept, b , satisfies:

$$b = \frac{7130 + 4580 + 2420 + 810}{4} - (-211.2)25$$
$$b = 9015$$

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Thus, the best fitting line is given by

$$c(t) = -211.2t + 9015$$

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With $c(t) = -211.2t + 9015$, compute the errors

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$$e_2 = c_2 - c(20) = 4580 - 4791 = -211$$

$$e_3 = c_3 - c(30) = 2420 - 2679 = -259$$

$$e_4 = c_4 - c(40) = 810 - 567 = 243$$

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The sum of the square of these errors is

$$J(-211.2, 9015) = 51529 + 44521 + 67081 + 59049 = 222180$$

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Least sum of square errors is found to be

$$J(m, b) = 41.5$$

Applet for Juvenile Height Growth

Example 1 - Model Choice

1

Two researchers had only a limited set of data,
the points $(2,2)$, $(5,6)$, and $(8,3)$.

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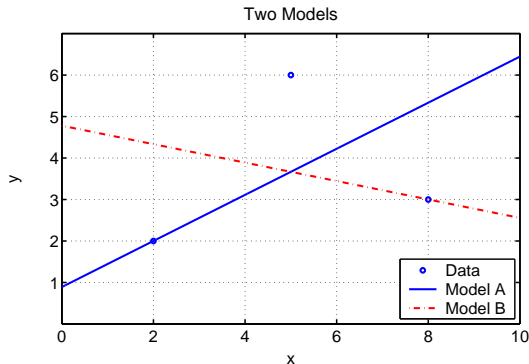
Researcher B felt that the model given by with y decreasing
with increasing x

$$y = -\frac{2}{9}x + \frac{43}{9}$$

Example 1

2

Graph of data and two models:



- Find the sum of square errors for each model
- Which one is better according to the data

Example 1

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Solution: Recall the error for line $y = ax + b$ satisfies:

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For **Model A**,

$$J_A = e_1^2 + e_2^2 + e_3^2$$

$$J_A = \left(2 - \left(\frac{5}{9}(2) + \frac{8}{9}\right)\right)^2 + \left(6 - \left(\frac{5}{9}(5) + \frac{8}{9}\right)\right)^2 + \left(3 - \left(\frac{5}{9}(8) + \frac{8}{9}\right)\right)^2$$

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$$J_A = 10.89$$

Example 1

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For Model B,

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For Model B,

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$$J_B = 10.89$$

Since $J_A = J_B$, the two models are equally valid

Example 1

5

What is the best fitting Linear model for these data?

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Solution: The average x is

$$\bar{x} = \frac{2+5+8}{3} = 5$$

Best slope a satisfies:

$$a = \frac{(2-5)2+(5-5)6+(8-5)3}{(2-5)^2+(5-5)^2+(8-5)^2} = \frac{1}{6}$$

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$$b = \bar{y} - a\bar{x} = \frac{11}{3} - \frac{5}{6} = \frac{17}{6}$$

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$$b = \bar{y} - a\bar{x} = \frac{11}{3} - \frac{5}{6} = \frac{17}{6}$$

The best linear model is

$$y = \frac{1}{6}x + \frac{17}{6}$$

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The sum of square error between the data and the best fitting model is **8.17**, which is better than other models (**10.89**)

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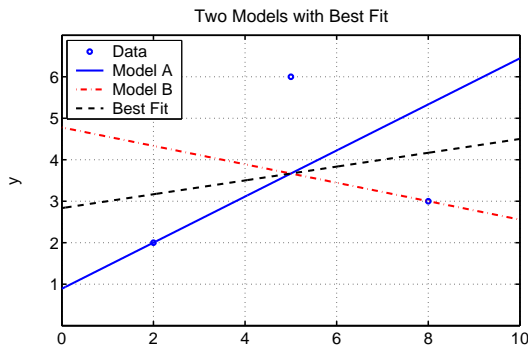
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Graph of data and three models:



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- The **Absolute Error** is appropriate when only the magnitude of the error is needed

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- The **Absolute Error** is appropriate when only the magnitude of the error is needed

$$\text{Percent Error} = \frac{X_e - X_t}{X_t} \times 100\%$$

Growth Model

Consider the growth of a fish given by the data:

t (weeks)	0	1	2	3	5	7	9
L (cm)	2.4	3.1	3.7	4.1	5.2	4.9	6.9

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Determine the growth rate for this model

Solution: The rate of growth is the slope of the best fitting line, so

Growth Rate = 0.437 cm/week

Growth Model

2

Find the sum of square errors

Growth Model

2

Find the sum of square errors

Solution: Each of the square errors is:

$$e_1^2 = (2.4 - 2.644)^2 = 0.0595$$

$$e_2^2 = [3.1 - (0.437 + 2.644)]^2 = 0.0004$$

$$e_3^2 = [3.7 - (0.874 + 2.644)]^2 = 0.0331$$

$$e_4^2 = [4.1 - (1.311 + 2.644)]^2 = 0.0210$$

$$e_5^2 = [5.2 - (2.185 + 2.644)]^2 = 0.1376$$

$$e_6^2 = [4.9 - (3.059 + 2.644)]^2 = 0.6448$$

$$e_7^2 = [6.9 - (3.933 + 2.644)]^2 = 0.1043$$

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$$e_6^2 = [4.9 - (3.059 + 2.644)]^2 = 0.6448$$

$$e_7^2 = [6.9 - (3.933 + 2.644)]^2 = 0.1043$$

Sum of Square Errors is

$$J(0.437, 2.644) = 1.0008$$

Growth Model

- Some data sets have points that are erroneous due to problems with the experiment (say contamination) or simply a poorly recorded value
- Statistical tests exist to determine if point can be removed
- Hypothesis testing studied in Bio 215
- If these points are included in the model, then they can result in misleading models

Growth Model

4

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Growth Model

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Which point is most likely erroneous?

The point with the most error is (7, 4.9)

When this point is removed, the new least squares best fit model is

$$L = 0.492t + 2.594$$

Determine the growth rate for this model

Growth Model

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Growth Rate = 0.492 cm/week

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What is the new sum of square errors

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What is the new sum of square errors

Solution: The new sum of square errors is

$$J(a, b) = 0.0376 + 0.0002 + 0.0149 + 0.0009 + 0.0213 + 0.0149 = 0.0898$$

Growth Model

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Solution: The new sum of square errors is

$$J(a, b) = 0.0376 + 0.0002 + 0.0149 + 0.0009 + 0.0213 + 0.0149 = 0.0898$$

which is only 9% of the sum of squares error from above

Growth Model

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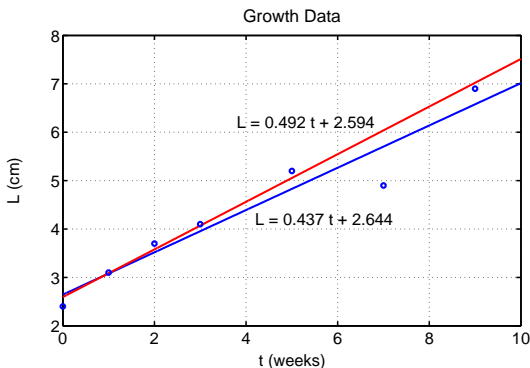
$$X_e = 0.437$$

Percent error is

$$\left(\frac{0.437 - 0.492}{0.492} \right) \times 100 = -11.2\%$$

Growth Model

Graph of data and two models:



Graph readily shows linear data and erroneous point