

CD-ROM Appendix A: Equal-Area Graphical Differentiation

There are many ways of differentiating numerical and graphical data. We shall confine our discussions to the technique of equal-area differentiation. In the procedure delineated below we want to find the derivative of y with respect to x .

1. Tabulate the (y_i, x_i) observations as shown in Table CDA-1.
2. For each *interval*, calculate $\Delta x_n = x_n - x_{n-1}$ and $\Delta y_n = y_n - y_{n-1}$.

TABLE CDA-1

x_i	y_i	Δx	Δy	$\frac{\Delta y}{\Delta x}$	$\frac{dy}{dx}$
x_1	y_1				$\left(\frac{dy}{dx}\right)_1$
		$x_2 - x_1$	$y_2 - y_1$	$\left(\frac{\Delta y}{\Delta x}\right)_2$	
x_2	y_2				$\left(\frac{dy}{dx}\right)_2$
		$x_3 - x_2$	$y_3 - y_2$	$\left(\frac{\Delta y}{\Delta x}\right)_3$	
x_3	y_3				$\left(\frac{dy}{dx}\right)_3$
		$x_4 - x_3$	$y_4 - y_3$	$\left(\frac{\Delta y}{\Delta x}\right)_4$	
x_4	y_4				$\left(\frac{dy}{dx}\right)_4$

TABLE CDA-1 (CONTINUED)

$x_5 - x_4$		$y_5 - y_4$	$\left(\frac{\Delta y}{\Delta x}\right)_5$
x_5	y_5	etc.	

3. Calculate $\Delta y_n/\Delta x_n$ as an estimate of the *average* slope in an interval x_{n-1} to x_n .
4. Plot these values as a histogram versus x_i . The value between x_2 and x_3 , for example, is $(y_3 - y_2)/(x_3 - x_2)$. Refer to Figure CDA-1.

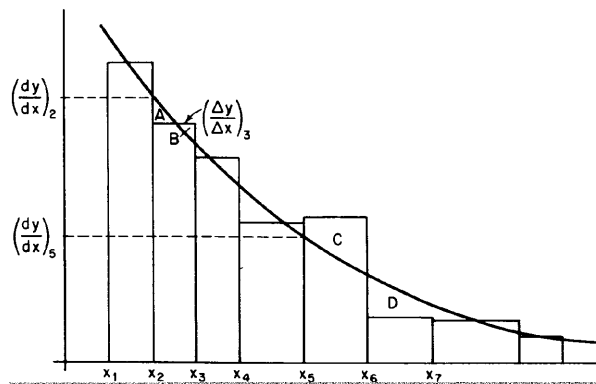


Figure CDA-5 Equal-area differentiation.

5. Next draw in the *smooth curve* that best approximates the *area* under the histogram. That is, attempt in each interval to balance areas such as those labeled A and B, but when this approximation is not possible, balance out over several intervals (as for the areas labeled C and D). From our definitions of Δx and Δy we know that

$$y_n - y_1 = \sum_{i=2}^n \frac{\Delta y}{\Delta x_i} \Delta x_i \quad (\text{A-19})$$

The equal-area method attempts to estimate dy/dx so that

$$y_n - y_1 = \int_{x_1}^{x_n} \frac{dy}{dx} dx \quad (\text{A-20})$$

that is, so that the area under $\Delta y/\Delta x$ is the same as that under dy/dx , *everywhere possible*.

6. Read estimates of dy/dx from this curve at the data points x_1, x_2, \dots and complete the table.

To illustrate this technique, consider the following data from which we wish to determine df/dx as a function of x :

x	0	0.2	0.4	0.6	0.8	1.0
$f(x)$	0	182	330	451	551	631

First we calculate $\Delta f/\Delta x$ (Table CDA-2) and then plot it in the manner shown in Figure CDA-6. After drawing the smooth equal-area curve, we can complete our table to find df/dx as a function of x (Table CDA-3).

TABLE CDA-2

x	$f(x)$	$\frac{\Delta f}{\Delta x}$
0	0	$\frac{182 - 0}{0.2 - 0} = 910$
0.2	182	$\frac{330 - 182}{0.40 - 0.2} = 740$
0.4	330	$\frac{451 - 330}{0.6 - 0.4} = 605$
0.6	451	$\frac{551 - 451}{0.8 - 0.6} = 500$
0.8	551	$\frac{631 - 551}{1.0 - 0.8} = 400$
1.0	631	

TABLE CDA-3

x	$f(x)$	$\frac{\Delta f}{\Delta x}$	$\frac{df}{dx}$	Actual $\frac{df}{dx}$
0	0	-	1010	1000
0.2	182	910	805	818
0.4	332	740	670	670
0.6	451	605	550	548
0.8	551	500	450	449
1.0	631	400	360	368

The function used in this example was

$$f(x) = 1000(1 - e^{-x}) \quad (\text{A-21})$$

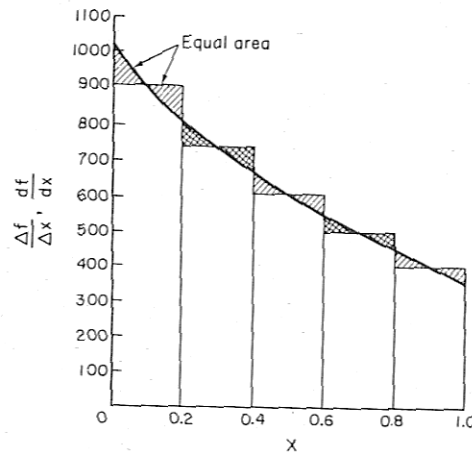


Figure CDA-6 Equal-area differentiation.

Differentiating equation (A-21) with respect to x gives us

$$\frac{df}{dx} = 1000e^{-x}$$

The actual numerical values of the differential are given in the last column of Table CDA-3.

Differentiation is, at best, less accurate than integration. This method also *clearly indicates bad data* and allows for compensation of such data. Differentiation is only valid, however, when data are presumed to differentiate *smoothly*, as in rate-data analysis and the interpretation of transient diffusion data.