RSC | Advancing the Chemical Sciences

Linear Function

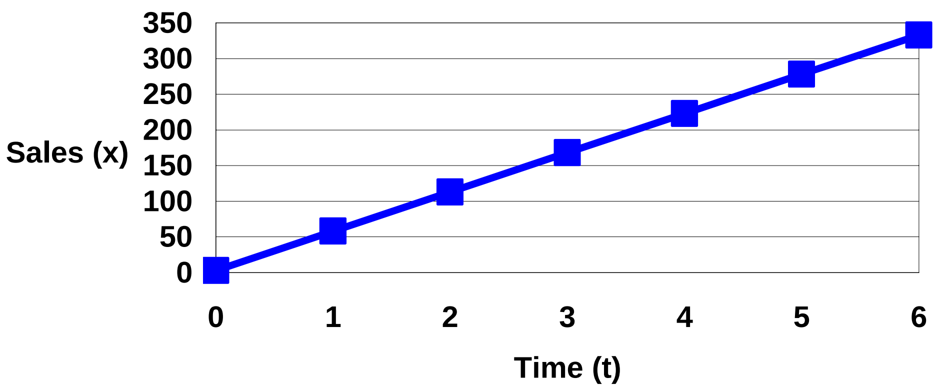
Consider a data series as shown in Table 1, how would you extrapolate the sales figures into time periods 7, 8 etc?

Table 1

Time (t)	0	1	2	3	4	5	6
Sales (x)	3	58	113	168	223	278	333

Plotting the sales figures onto a graph shows that the trend is linear in nature therefore the trend may be represented by a linear function.

$$x = a_0 + a_1 t$$



For a linear function the coefficient $\mathbf{a_0}$ is the intersection on the sales axis and the coefficient $\mathbf{a_1}$ is the gradient of the linear graph.

Hence:

$$x = 3 + 55t$$

So to predict the future for time periods 7 and 8 using the linear trend, solve the equation for ***t*** = 7 and ***t*** = 8 etc.

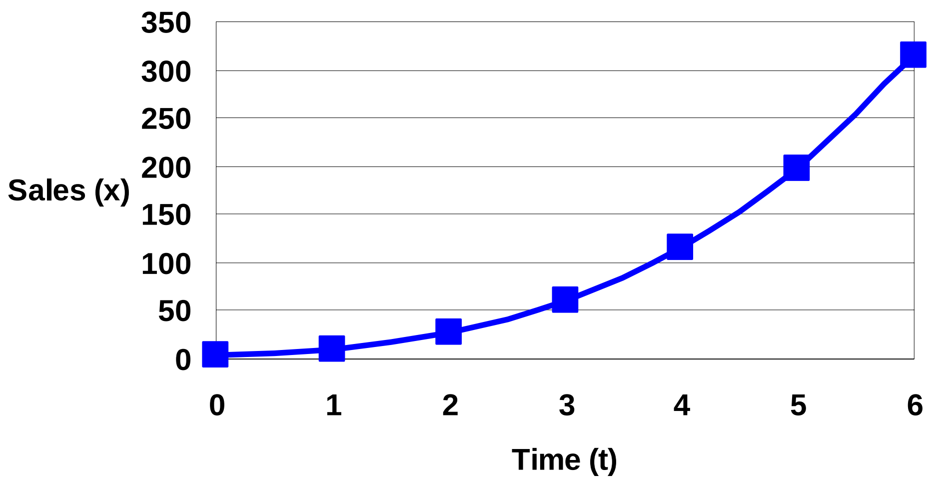
Polynomial Function

Consider a data series as shown in Table 2

Table 2

Time (t)	0	1	2	3	4	5	6
Sales (x)	3	10	27	60	115	198	315

Plotting the sales figures onto a graph shows that the sales start to rise slowly and then gradually increase more quickly.



This trend is typical of a polynomial function, which is represented by the equation:.

$$x = a_0 + a_1 t + a_2 t^2 + ... + a_n t^n$$

The highest power level of **n** may be determined by a process of repeating differences. Table 2a shows the original sales figures expressed vertically. Column 3 shows the difference in the sales between a time period and the previous time period, so for time period t = 1 then the 1st difference is 10-3 = 7, for t = 2 the 1st difference is 27-10 = 17 etc. Column 4 shows the 2nd difference, so for time period t = 2 the 2nd difference is 17-7 = 10 etc. Column 5 shows the 3rd difference and column 6 shows the 4th difference. Differences are calculated until they are all very similar in value or in the next column they are all close to zero. In this case the 3rd difference table shows all similar values so the highest power value of **n** is 3. Variation within the data will mean that this procedure is never perfect but it should indicate an appropriate power level to use. Computer regression packages may be used to derive the best fit binomial expression automatically.

Table 2a

Time (t)	Sales (x)	1st difference	2nd difference	3rd difference	4th difference
0	3				
1	10	7			
2	27	17	10		
3	60	33	16	6	
4	115	55	22	6	0
5	198	83	28	6	0
6	315	117	34	6	0

Therefore the most appropriate general binomial equation is: $x = a_0 + a_1 t + a_2 t^2 + a_3 t^3$

The coefficients may be solved by preparing simultaneous equations:

At t = 0 , x = 3 so $3 = a_0$
At t = 1 , x = 10 so $10 = 3 + a_1 + a_2 + a_3$
At t = 2 , x = 27 so $27 = 3 + 2a_1 + 4a_2 + 8a_3$
At t = 3 , x = 60 so $60 = 3 + 3a_1 + 9a_2 + 27a_3$

Hence solving the simultaneous equations will give the values of the coefficients

$$x = 3 + 4t + 2t^2 + t^3$$

So to predict the future for time periods 7 and 8 using the polynomial trend solve the equation for ***t*** = 7 and ***t*** = 8 etc.

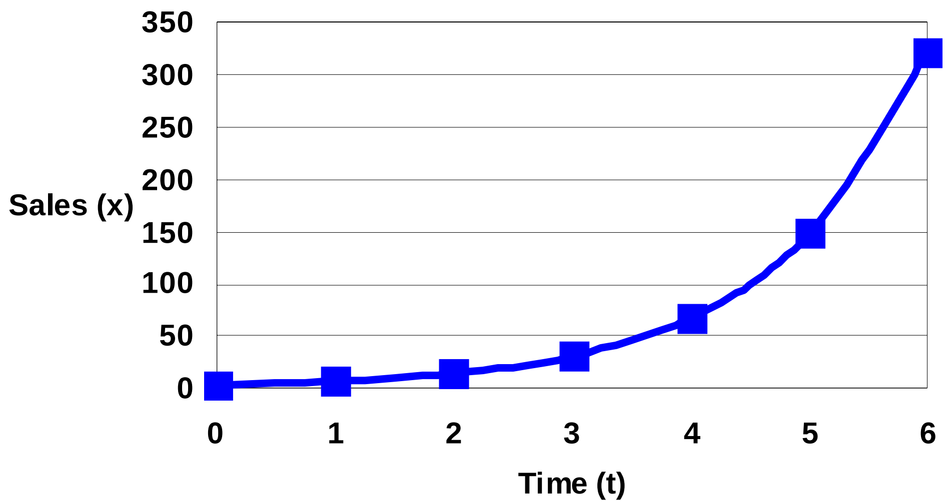
Exponential Function

Consider a data series as shown in Table 3

Table 3

Time (*t*)	0	1	2	3	4	5	6
Sales (*x*)	3	6.5	14	31	68	148	323

Plotting the sales figures onto a graph shows that the sales start to rise slowly and then rapidly increase more quickly. The exponential trend is similar in shape to the binomial trend but tends to be used when the rise in sales is more rapid.



This trend is typical of an exponential function, which is represented by the equation:.

$$x = x_0 e^{rt}$$

You will have come across a similar equation as a first order kinetic rate equation or radioactive decay. The value of $\mathbf{x_0}$ may be determined from the intersection on the sales axis at time **t** = 0 and the growth constant **r** be determined from slope a graph of ln ***x*** against ***t*** .

Hence the exponential equation is:

$$x = 3e^{0.78t}$$

So to predict the future for time periods 7 and 8 using the exponential trend solve the equation for ***t*** = 7 and ***t*** = 8 etc.

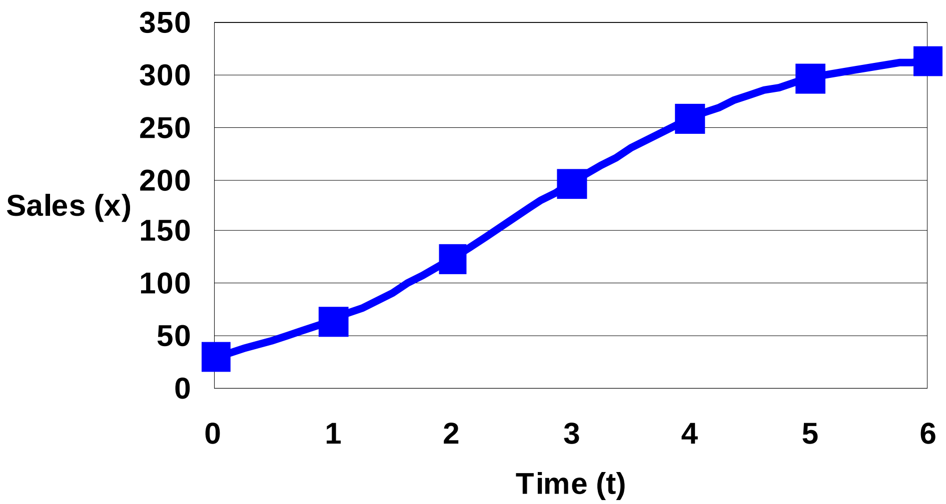
Logistic Function

Consider a data series as shown in Table 4

Table 4

Time (t)	0	1	2	3	4	5	6
Sales (x)	30	65	124	197	259	297	316

Plotting the sales figures onto a graph shows that the sales start to rise slowly then much faster then they tail off to eventually reach a saturation point.



This trend is typical of a exponential function, which is represented by the equation:.

$$x = \frac{k}{\left(1 + be^{-rt}\right)}$$

A logistic trend may be used to represent a S-shaped curve.

The coefficients may be determined by plotting a graph of $(1/\boldsymbol{x})(d\boldsymbol{x}/d\boldsymbol{t})$ versus $\boldsymbol{x}$ which will be a straight line with a slope -r/k and intercept r. A value for 1/b may be estimated from average values of $\boldsymbol{x}\, e^{(-r\boldsymbol{t})} / (k-\boldsymbol{x})$.

Hence the logistic equation is:

$$x = \frac{330}{\left(1 + 10e^{-0.9t}\right)}$$