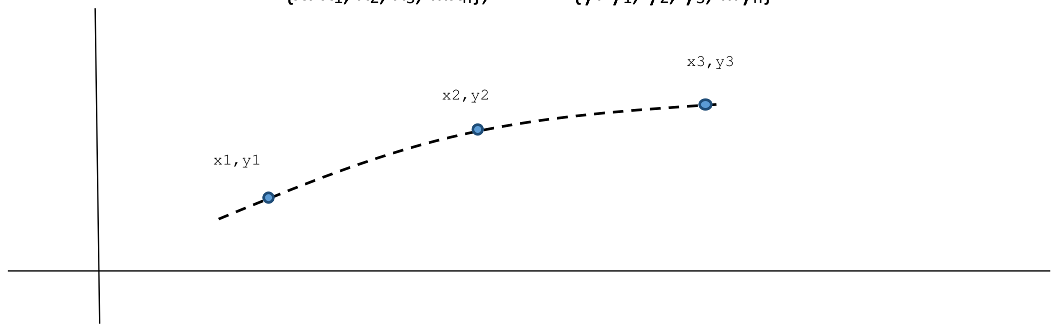
Numerical Differentiation

For a programmer data is usually discrete. It either exists in arrays or has been recorded at (regular) intervals:

$\{x: x_1, x_2, x_3, \ldots x_n\}$; $\{y: y_1, y_2, y_3, \ldots y_n\}$



A derivative is simply a slope and since $(y_2-y_1)/(x_2-x_1)$ is a slope, is it also a derivative? The answer is yes, but not a very good one because it's not the slope at (x_1,y_1) and it's not the slope at (x_2,y_2); it most accurately represents the slope half-way between them, but there isn't a data point there!
To get a general result for the derivatives at data points we consider a Maclaurin function for the notional curve, represented by the dotted curve, above, that passes through the data points. To make the result general we consider three general adjacent data points (x_{i-1},y_{i-1}), (x_i,y_i), (x_{i+1},y_{i+1}) separated by $\Delta x = x_{i+1}-x_i = x_i-x_{i-1}$.

1. The Maclaurin function going forward from x_i to x_{i+1} is

$$y_{i+1} = y_i + \frac{dy}{dx_i}.\Delta x + \frac{d^2y}{dx^2{}_i}\frac{\Delta x^2}{2!} + \frac{d^3y}{dx^3{}_i}\frac{\Delta x^3}{3!} + O(\Delta x^4) + .. \qquad 1.$$

2. The Maclaurin function going backward from x_i to x_{i-1} is

$$y_{i-1} = y_i + \frac{dy}{dx_i}.(-\Delta x) + \frac{d^2y}{dx^2{}_i}\frac{(-\Delta x)^2}{2} + \frac{d^3y}{dx^3{}_i}\frac{(-\Delta x)^3}{3!} + O(\Delta x4) + \cdots$$

$$y_{i-1} = y_i - \frac{dy}{dx_i}.\Delta x + \frac{d^2y}{dx^2{}_i}\frac{\Delta x^2}{2} - \frac{d^3y}{dx^3{}_i}\frac{\Delta x^3}{3!} + O(\Delta x^4)\ldots \qquad 2.$$

1st Derivative

Subtracting 1. – 2. $\quad y_{i+1} - y_{i-1} = 2\,\frac{dy}{dx_i}\,\Delta x + 2\frac{d^3y}{dx^3{}_i}\frac{\Delta x^3}{3!} + O(\Delta x^5) + ..$

Solving for the first derivative and neglecting terms $O(\Delta x^3)$ and higher we get: $\frac{dy}{dx_i} = \frac{y_{i+1}-y_{i-1}}{2\Delta x}$

This result is called the Centered Divided Difference First Derivative. It is accurate to $O(\Delta x^3)$, which means the error appears at order Δx^3.

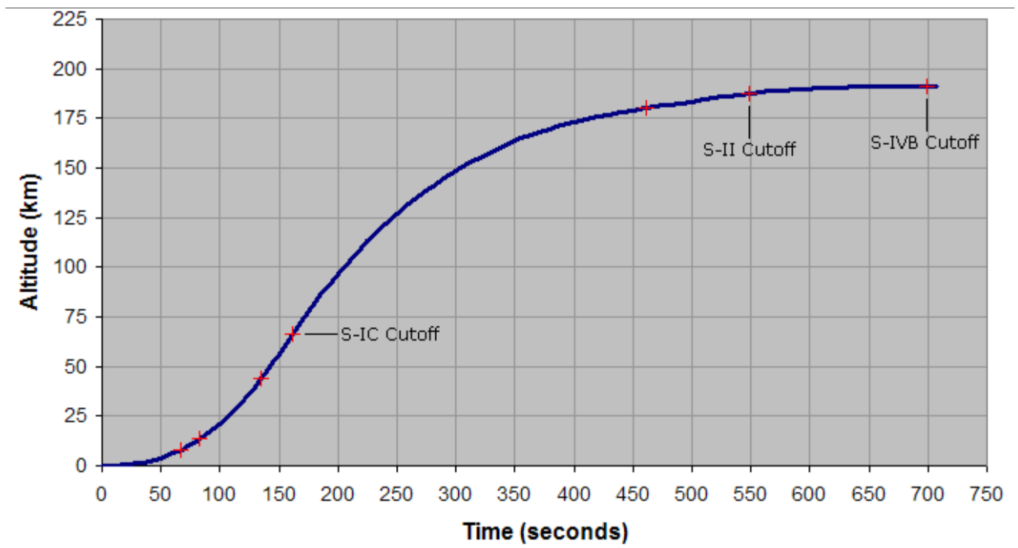
2nd Derivative

Adding 1. + 2. $\quad y_{i+1} + y_{i-1} = 2y_i + \frac{d^2y}{dx^2{}_i}\Delta x^2 + O(\Delta x^4) + \ldots$

Solving for the second derivative and neglecting terms $O(\Delta x^4)$ and higher we get: $\frac{d^2y}{dx^2{}_i} = \frac{y_{i+1}+y_{i-1}-2y_i}{\Delta x^2}$

This result is called the Centered Divided Difference Second Derivative. It is accurate to $O(\Delta x^4)$, which means the error appears at order Δx^4.
We can estimate the relative sizes of the neglected terms. For example if $\Delta x \sim 0.1$, then $\Delta x^2 \sim 0.01$, $\Delta x^3 \sim 0.001$ and $\Delta x^4 \sim 0.0001$, and the increasing factorials in the denominators will make them even smaller. In this case the neglected terms become relatively small very fast.

Example. The following data are from the launch of Apollo 11 on 16 july 1969. They show the altitude (km) with time (seconds) after the launch:



The following data for the height at regular intervals is taken from the graph.

t sec	0	25	50	75	100	125	150	175	200	225	250	275	300	325	350	375	400	425	450
height km	0	1	4	10	20	38	57	78	97	113	127	138	148	158	163	170	174	176	178

Qu 1. Calculate the vertical velocity in m/sec with time

The vertical velocity v is the first derivative of the vertical height:

$$v = \frac{dh}{dt}$$

It can be calculated as the first derivative of the height with time using the First Derivative Divided Difference formula and the data in the table:

t sec	0	25	50	75	100	125	150	175	200	225	250	275	300	325	350	375	400	425	450
height km	0	1	4	10	20	38	57	78	97	113	127	138	148	158	163	170	174	176	178

t sec	0	25	50	75	100	125	150	175	200	225	250	275	300	325	350	375	400	425	450
v m/sec	0	80	180	320	560	740	800	800	700	600	500	420	400	300	240	220	120	80	-

Qu 2. Calculate the vertical acceleration in m/sec^2 with time

The vertical acceleration a is the second derivative of the vertical height:

$$a = \frac{d^2h}{dt^2}$$

It can be calculated as the second derivative of the height with time using the Second Derivative Divided Difference formula and the data in the table:

t sec	0	25	50	75	100	125	150	175	200	225	250	275	300	325	350	375	400	425	450
height km	0	1	4	10	20	38	57	78	97	113	127	138	148	158	163	170	174	176	178

t sec	0	25	50	75	100	125	150	175	200	225	250	275	300	325	350	375	400	425	450
accn m/sec^2	-	3.2	4.8	6.4	12.8	1.6	3.2	-3.2	-4.8	-3.2	-4.8	-1.6	0.0	-8	3.2	-4.8	-3.2	0.0	-

(Note that although acceleration is the first derivative of velocity, we do not use the calculated velocities and the first divided difference formula to calculate the acceleration. It is more accurate to use the second divided difference formula on the original distance data directly).