Scientific Computing in Python Lecture 1

Python and sampled measurements

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Values and assignment

```
a = 4
b = 2*a
a = 7
```

The final values are $a = 7$ and $b = 8$. The second line was evaluated before the third.

Expression evaluation

```
x = 3
print(x**2 + 1)  # 10
print((x + 1)**2)  # 16
```

Exponentiation uses **. Parentheses determine which quantity is squared.

Paired observations

$$(t_i, T_i) = (0, 80), (60, 62), (120, 48), (180, 38), (240, 31).$$

Time is in seconds and temperature in degrees Celsius.

```
time_seconds = [0, 60, 120, 180, 240]
temperature_c = [80, 62, 48, 38, 31]
```

Indexing the endpoints

```
t0 = time_seconds[0]
t1 = time_seconds[-1]
T0 = temperature_c[0]
T1 = temperature_c[-1]
```

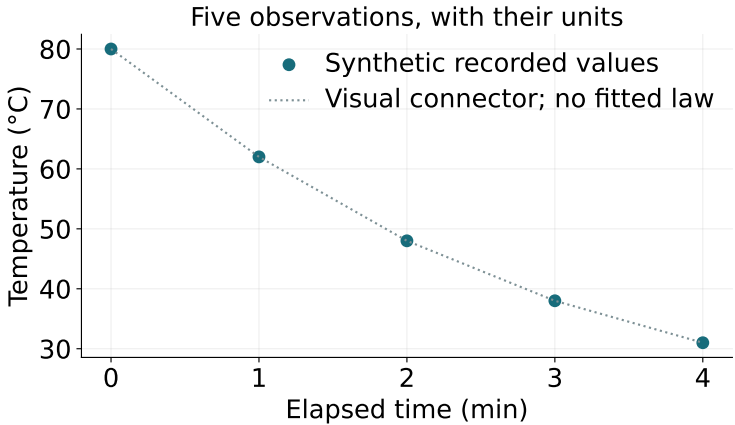
The endpoint calculation uses $(0, 80)$ and $(240, 31)$. Interior observations remain relevant to the plotted record.

Units and affine changes of scale

$$t_{\mathrm{min}} = \frac{t_{\mathrm{s}}}{60}, \qquad T_K = T_C + 273.15.$$

$$\Delta T_K = (T_{C,1} + 273.15) - (T_{C,0} + 273.15) = \Delta T_C.$$

The sampled temperature record



The same change in two units

$$\Delta T = 31 - 80 = -49\ ^\circ\mathrm{C} = -49\ \mathrm{K}.$$

$$\Delta t = 240\ \mathrm{s} = 4\ \mathrm{min}.$$

Temperature differences have equal numerical values in Celsius and kelvin. Absolute temperatures do not.

Average rate of change

$$\overline{r} = \frac{T_1 - T_0}{t_1 - t_0}, \qquad t_1 > t_0.$$

$$\overline{r} = \frac{-49}{4} = -12.25\ ^\circ\mathrm{C/min}.$$

This is an interval average, not an instantaneous derivative.

A direct Python calculation

```
elapsed_min = (time_seconds[-1]-time_seconds[0])/60
change_c = temperature_c[-1]-temperature_c[0]
rate_c_per_min = change_c/elapsed_min
```

A zero elapsed time would make the quotient undefined. The denominator must be checked before division.

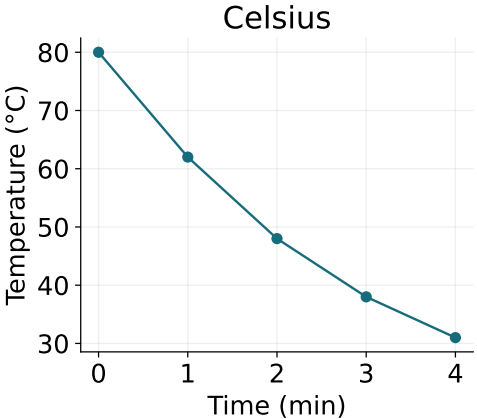
Floating-point arithmetic

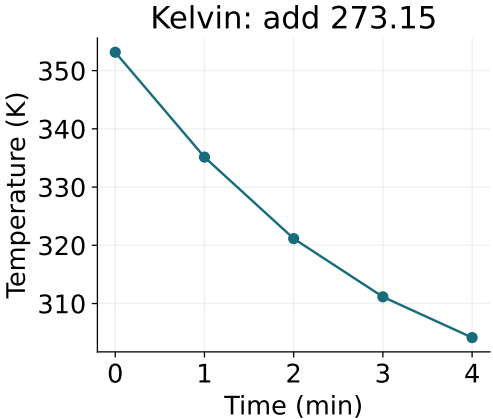
```
0.1 + 0.2 == 0.3  # False in binary floating point
```

A useful comparison has the form

$$|a - b| \leq \varepsilon_{\text{abs}} + \varepsilon_{\text{rel}}|b|.$$

Celsius and kelvin





Scale in an error tolerance

The absolute term controls comparisons near zero. The relative term scales with the reference magnitude.

$$|60r_{\mathrm{s}} - r_{\mathrm{min}}| \leq 10^{-12}$$

is a numerical unit-conversion check for this small example. It is not a statement about thermometer accuracy.

Plots and reproducible execution

Five observations determine five plotted points. They do not determine the complete function $T(t)$. If $g(t_i) = 0$ at every sampled time, both $T(t)$ and $T(t) + g(t)$ fit those observations.

A family of indistinguishable interpolants

For any constant c,

$$g(t) = c \prod_{i=0}^{4} (t - t_i)$$

vanishes at all five sample times. Additional assumptions are required to infer behavior between observations.