MCEN 3030

2 Apr 2024

Exam #2 Thurs 4 Apr

No HW Due Monday

Today: Numerical Derivatives

→ ODEs

→ PDEs

Taylor Series is maybe the most important idea in engineering analysis

- Newton's Method

  roots of an equation determined via implementation of $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$ ← rearranged Taylor Series

- Modified to a 2D Newton's method using a 2D Taylor Series

- Nonlinear Least Squares

  Adjust the best guess for parameters based on

$$\underbrace{\hat{f}(\alpha_i)}_{\text{to improve accuracy of model prediction}} = f(\alpha_i) + \frac{\partial f}{\partial \alpha}\bigg|_{\alpha_1} \cdot \underbrace{(\alpha_{i+1} - \alpha_i)}_{\text{how to adjust parameter } \alpha}$$

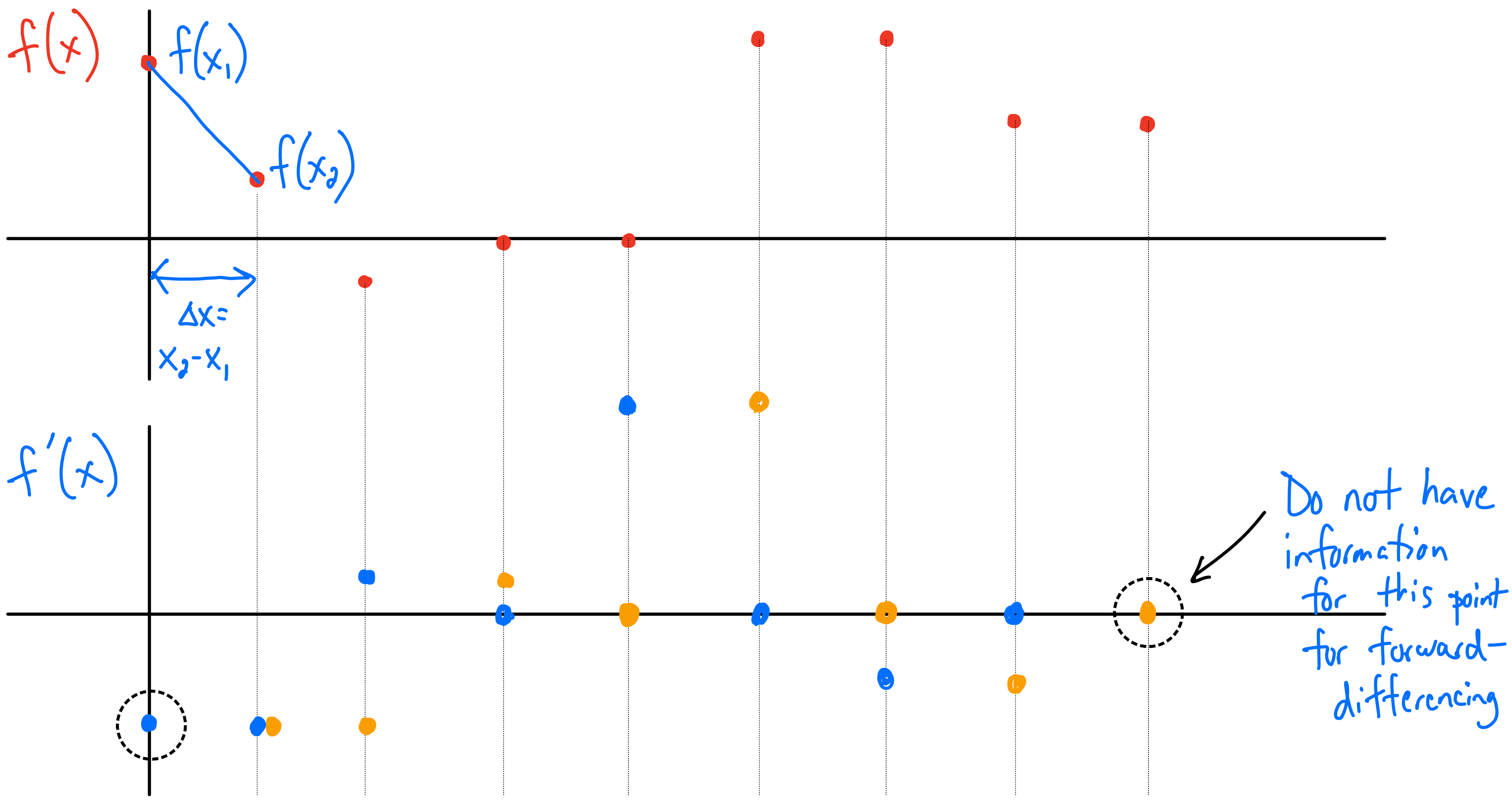
- Another application today, to get a numerical approximation of a derivative

Numerical Derivatives

Goal: To approximate the value of a derivative at a point based on data or a discrete set of points for a known/hypothetical function

For data: one approach is "forward-differencing"

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$



or backwards-differencing or central-differencing (not included above)

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$

What about the second derivative?

$$\left.\frac{d^2f}{dx^2}\right|_{x_i} \approx \frac{\left.\frac{df}{dx}\right|_{x_{i+1}} - \left.\frac{df}{dx}\right|_{x_i}}{x_{i+1} - x_i}$$ ⟵ call this Δx (uniform)

for forward difference

$$= \frac{\frac{f(x_{i+2}) - f(x_{i+1})}{\Delta x} - \frac{f(x_{i+1}) - f(x_i)}{\Delta x}}{\Delta x}$$

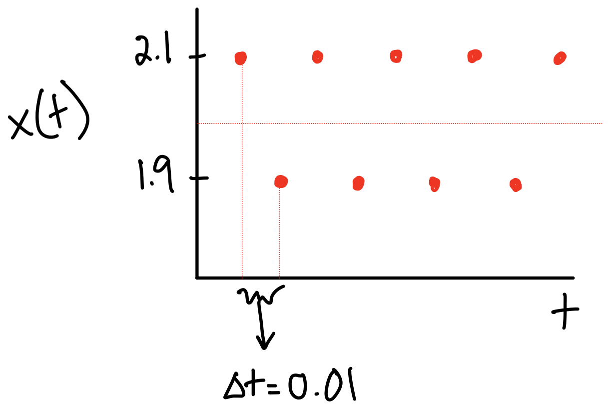
$$\left.\frac{d^2f}{dx^2}\right|_{x_i} \approx \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2}$$ forward diff

& similar for...

$$\left.\frac{d^2f}{dx^2}\right|_{x_i} \approx \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{(\Delta x)^2}$$ backwards diff

$$\left.\frac{d^2f}{dx^2}\right|_{x_i} \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2}$$ central diff

There is a danger with numerical differentiation of data that "noise"/error is magnified, e.g.



$\Longrightarrow$ 5% error in measurement from nominally constant position $x = 2$

What is the velocity?

forward diff

$$\left.\frac{dx}{dt}\right|_{i=1} \approx \frac{1.9-2.1}{0.01} = -20 \qquad \left.\frac{dx}{dt}\right|_{i=2} \approx 20 \quad \text{etc.}$$

& the acceleration?

forward diff

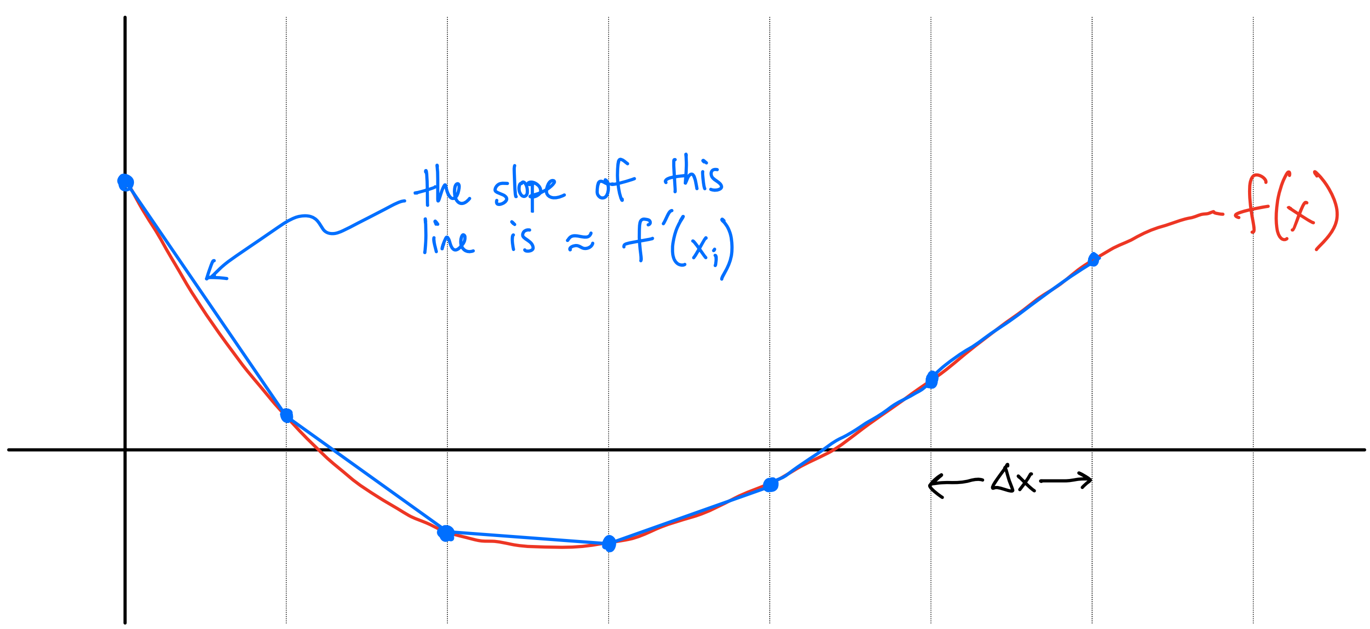
$$\left.\frac{d^2x}{dt^2}\right|_{i=1} \approx \frac{f(x_3)-2f(x_2)+f(x_1)}{(\Delta t)^2} = \frac{(2.1)-2(1.9)+(2.1)}{(0.01)^2} = 4000$$

So, a position measurement that was constant, with some error, implied a rapidly oscillating velocity, corresponding to an insane acceleration.

for a function can do similar based on Taylor Series

$$f(x_{i+1}) \approx \underbrace{f(x_i) + \left.\frac{df}{dx}\right|_{x_i} \cdot (x_{i+1} - x_i)}_{\text{for a small departure, we are often happy with the "linearization"}} + \frac{1}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_i} \cdot (x_{i+1} - x_i)^2 + \ldots$$

Rearrange $\longrightarrow$ $$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_{i+1}) - f(x_i)}{\Delta x}$$



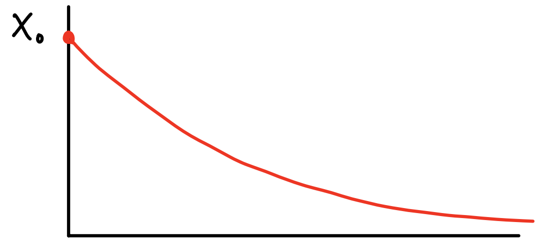
This approach can be used to numerically solve differential equations

simple example (that can run into issues!)

$$\frac{dx}{dt} = -ax$$

w/ $x(0) = x_0$

act like we don't know $x(t) = x_0 e^{-at}$

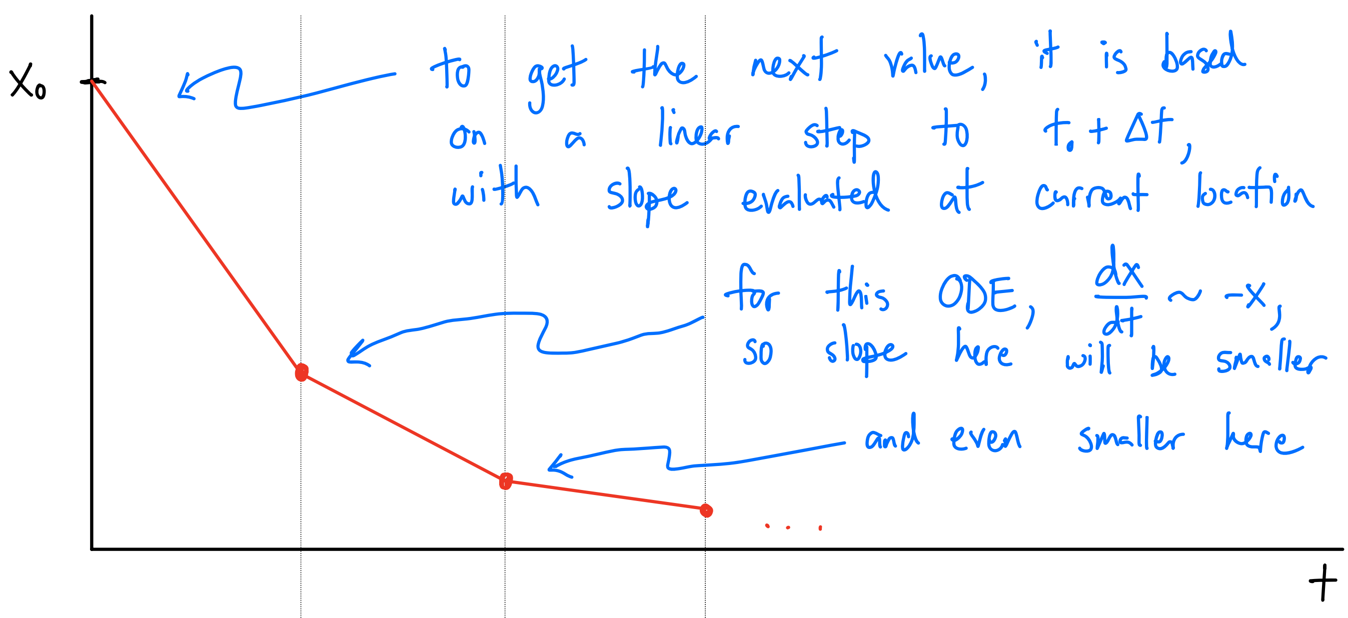


$$\frac{x(t_{i+1}) - x(t_i)}{\Delta t} = -a\,x(t_i)$$

$\Delta t = t_{i+1} - t_i$

→ rearrange : $x(t_{i+1}) = \underbrace{x(t_i) - \Delta t \cdot a\, x(t_i)}_{\text{known at current time step}}$

idea then is to construct a solution out to any time by stepping through values of i



to get the next value, it is based on a linear step to $t_0 + \Delta t$, with slope evaluated at current location

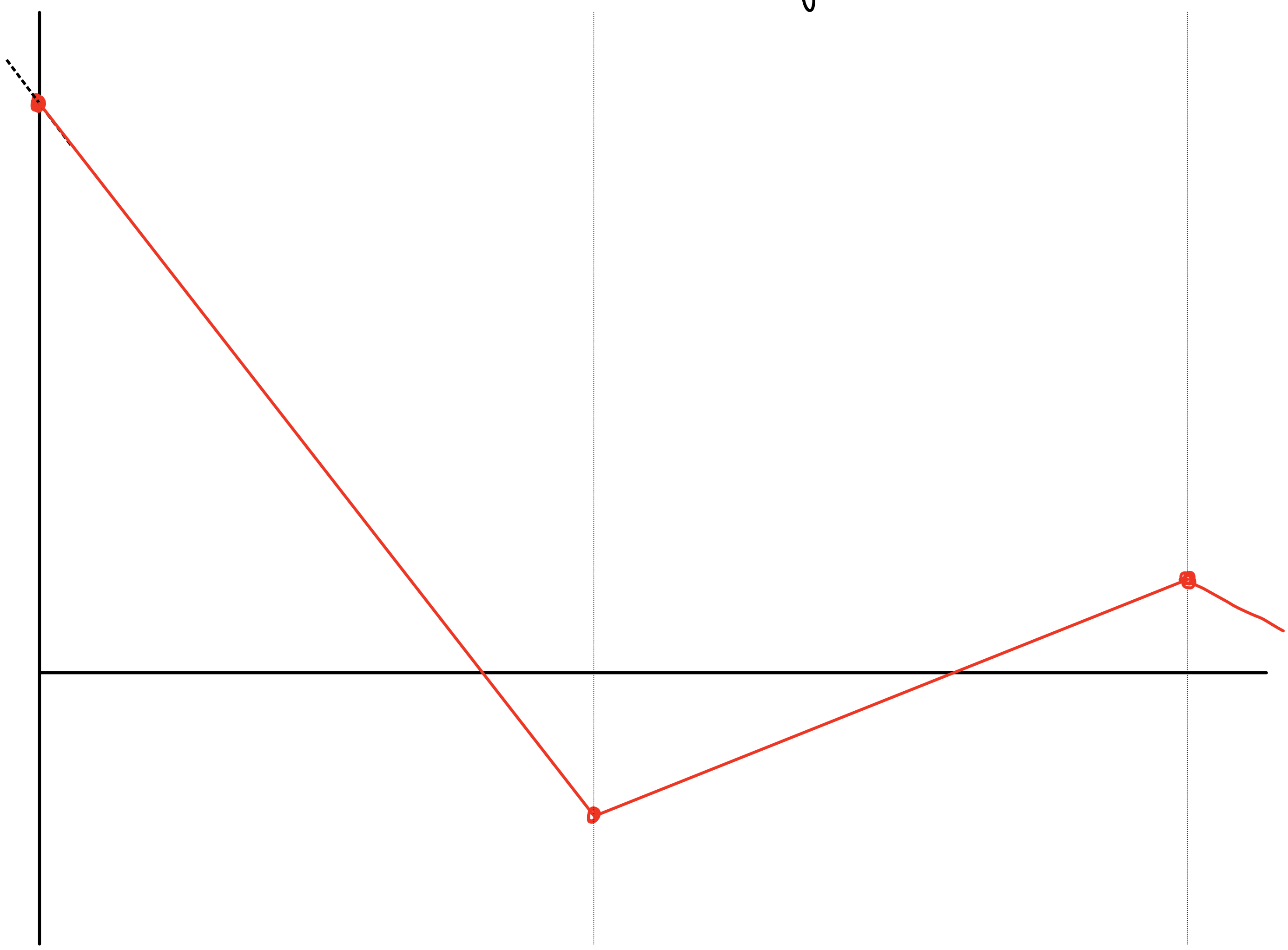
for this ODE, $\frac{dx}{dt} \sim -x$, so slope here will be smaller

and even smaller here

The above is known as <u>Euler's Method</u> for numerically solving ODEs.

We will talk more about error/stability of this method and variations, but a quick comment:

What if Δt is "too large"



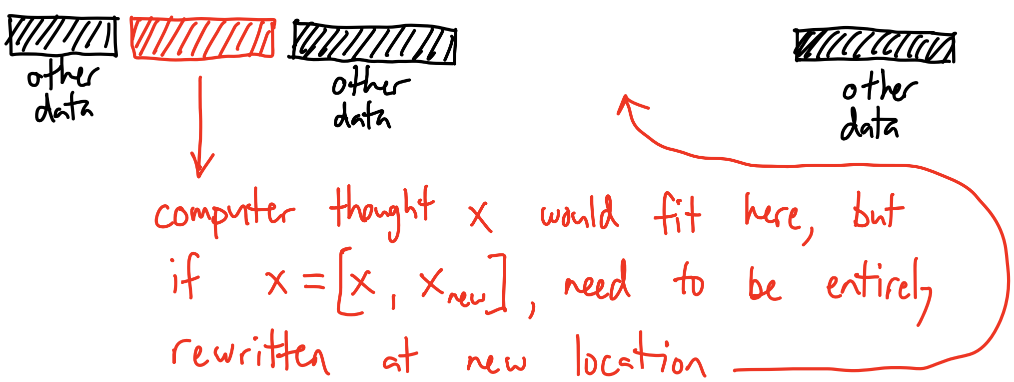
→ The solution should be $x(t) > 0$ for <u>all time</u>, but we predict otherwise

→ In general, smaller Δt means more accurate solution, but smaller $\Delta t \Rightarrow$ more computing time to reach t_{final}

On that topic, how to determine t_{final}?

- Maybe your problem has a known ending time, at least approximately.
  - E.g. "determine the position after 2 seconds"
  - or "how far does the ball travel?" ... and you know the flight time is <10 seconds, surely.

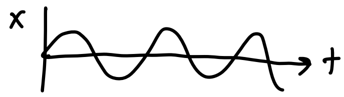
- With small problems on modern computers, it is not unreasonable to repeatedly append to a vector and monitor a convergence condition (if one is known).
  - MATLAB could do $x = [x, x_{next}]$ & $t = [t, t_{next}]$. The issue is that each time you do this, you need to find a new storage location because the size of the data has changed



* Pre-allocating space is generally better practice

$$t = 0 : \Delta t : t_{final};$$
$$x = zeros(size(t));$$

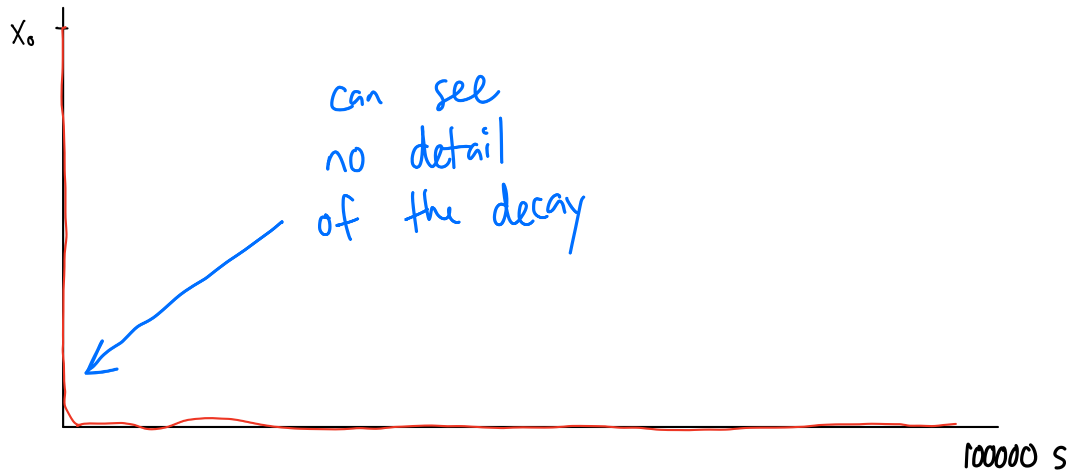
- Sometimes you don't need to store the entire history of data, e.g. if continuously responding to new input data: monitoring chlorine % in drinking water and adapting feed rate
- Sometimes there is no termination condition, e.g. $\frac{dx}{dt} = \cos t$



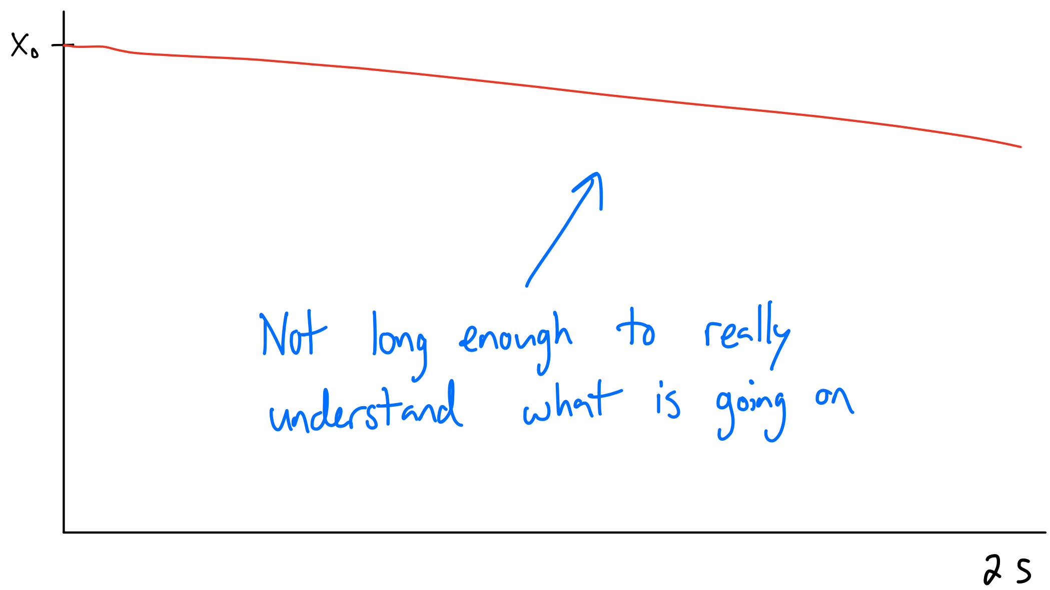
so... gotta decide when to stop.

- Sometimes choosing an inappropriate t_{final} leads to misleading results, e.g.

"I'll just choose something big"

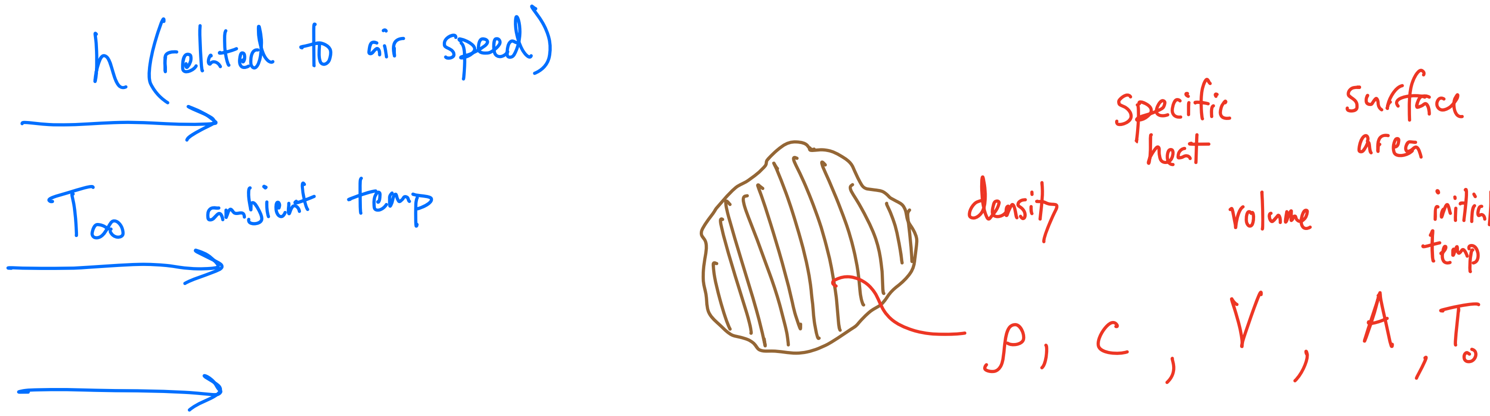


"Let's just choose 2 s or something"



Non-dimensionalization of governing equations

Useful for several reasons, explained later, but let's just dive in with an explanatory example



Fan-cool a meatball. Want to know $T(t)$ such that we can not burn our mouths, but also aren't eating a cold chunk of meat/beyond meat.

$$\dot{Q} = mc\frac{dT}{dt} = -hA(T - T_\infty)$$

$$\Rightarrow \frac{dT}{dt} = -\frac{hA}{\rho V c}(T - T_\infty) \qquad \text{w/ } T(0) = T_0$$

Apparently the behavior depends on 7 parameters,

$$h \quad A \overset{?}{\longleftrightarrow} V \quad \rho \quad c \quad T_0 \quad T_\infty$$

so to fully understand $T(t)$, need to test so many cases. E.g. if each variable has 5 possible variations ($T_\infty = 10, 15, 20, 25, 30°C$) there are $5^7 = 78{,}125$ combinations. And we don't know t_{final}, so naively could do $\Delta t = 0.01$ s, $t_{final} = 10000$ s $= 166.7$ min.

→ "That should be good enough."

→ I think this data set would be ~625 gigabytes in total.

Alternative approach: Do some pencil-and-paper work ahead of time

Non-dimensionalize the equation.

In this case we might be wise and will recognize

$$\frac{d}{dt}(T - T_\infty) = \frac{dT}{dt}$$

Then we suppose the existence of <u>characteristic values</u>, to be determined, such that we can define dimensionless variables $\Theta(\tau)$ (transformation of $T(t)$), with the goal of $|\Theta| \lesssim 1$ and $|\tau| \lesssim 1$ (or some small number, maybe 10 to be safe

$$\Theta = \frac{T - T_\infty}{(T_c - T_\infty)} \qquad \tau = \frac{t}{t_c}$$

constant to-be determined

constant to-be determined

$$\Downarrow \qquad\qquad \Downarrow$$

$$T = \Theta(T_c - T_\infty) + T_\infty \qquad t = t_c \tau$$

Plug these in:

$$\frac{d}{dt}\left(\theta\left(T_c - T_\infty\right) + T_\infty\right) = -\frac{hA}{\rho V c}\theta\left(T_c - T_\infty\right)$$

$$\cancel{\left(T_c - T_\infty\right)}\frac{d\theta}{dt} = -\frac{hA}{\rho V c}\theta\cancel{\left(T_c - T_\infty\right)}$$

need chain rule to get this in terms of τ

$$\frac{d\theta}{dt} = \frac{d\tau}{dt}\frac{d\theta}{d\tau} = \frac{1}{t_c}\frac{d\theta}{d\tau}$$

$$\therefore \frac{1}{t_c}\frac{d\theta}{d\tau} = -\frac{hA}{mc}\theta$$

choose $\frac{1}{t_c} = \frac{hA}{\rho V c}$ for convenience

Our problem becomes: $\frac{d\theta}{d\tau} = -\theta$

and we can choose $T_c = T_0$, again for convenience, such that

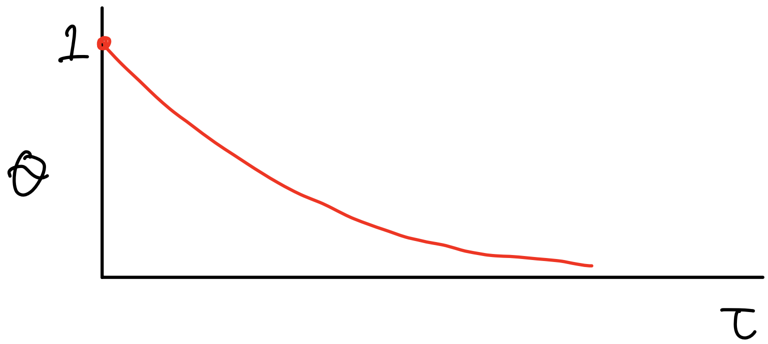
$$T(t=0) = T_0 \Longrightarrow \theta(0)\left(T_c - T_\infty\right) + T_\infty = T_0$$

$\tau = 0 \Leftrightarrow t = 0$

If $T_c = T_0 \longrightarrow \theta(\tau = 0) = 1$

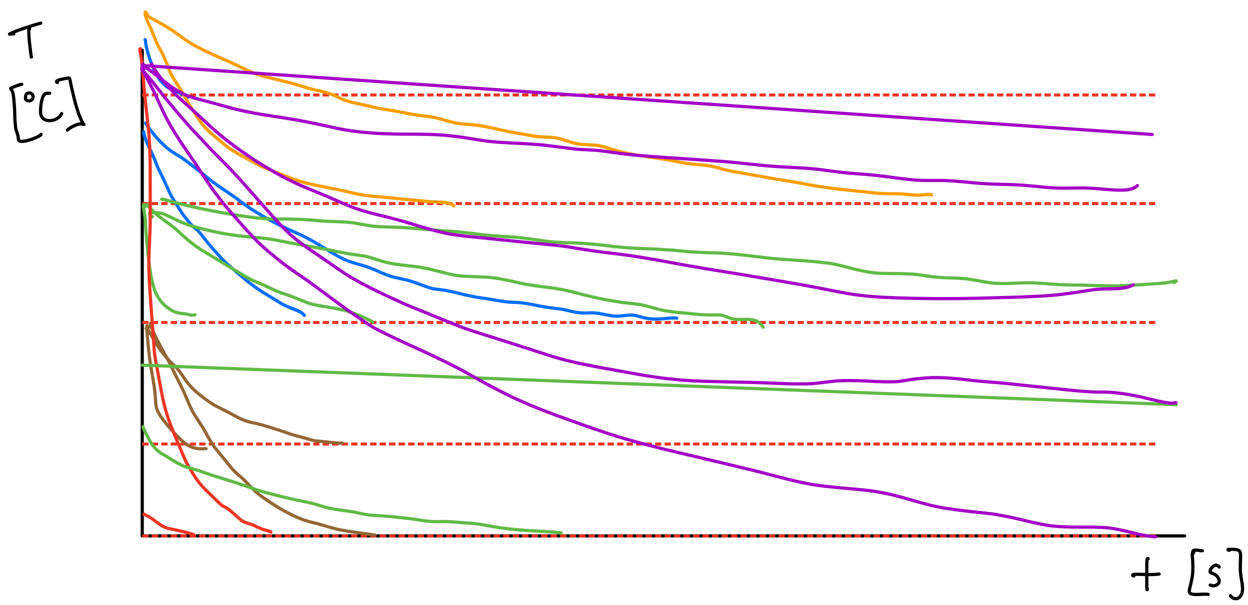
So we have $\dfrac{d\Theta}{d\tau} = -\Theta$ w/ $\Theta(0) = 1$

1) As we solve this equation, there are <u>no</u> parameters – we can apply to any specific situation by "unpacking" $\tau = \dfrac{hA}{\rho V c} t_c$. This means this one curve



applies to all combinations of $h, A, V, \rho, c, T_0, T_\infty$.

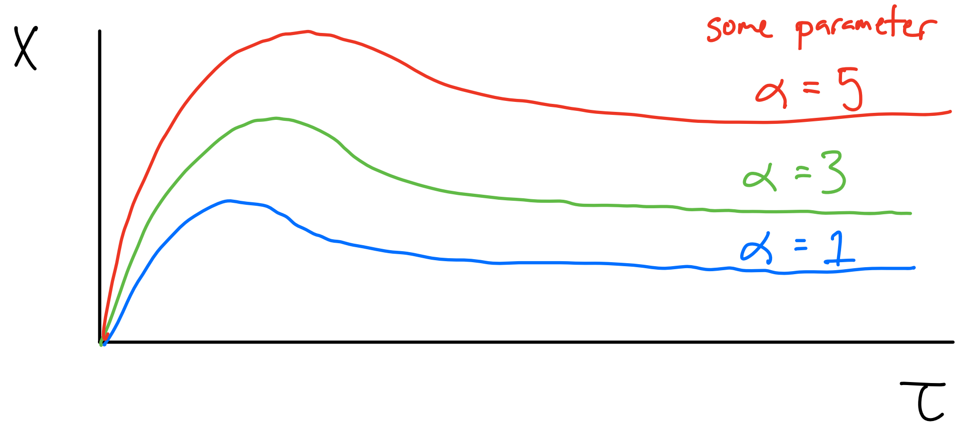
Compare against:



Good luck reading this chart and getting anything useful from it!

- In some problems there will be another parameter, but it is always fewer parameters than in the dimensional problem. (Buckingham - Π Theorem)

e.g



2) It is often safe to assume all the action of a problem will occur within small values of τ, e.g. 10, so $\tau_{final} = 10$ is probably a safe bet.

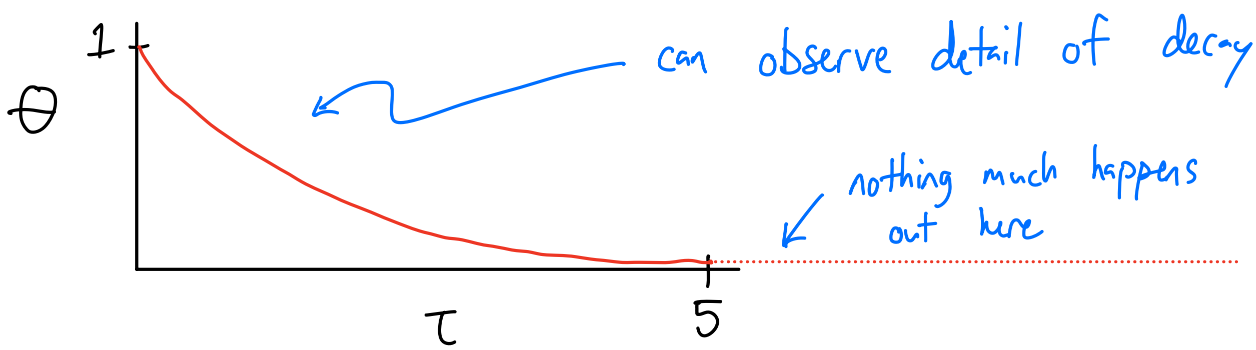
- In this problem

$$\theta(0) = 1, \quad \theta(1) = 0.37 \quad \& \quad \theta(10) = 0.00005$$

so $\quad 0 \leq \tau \lesssim 3$

& $\quad 0 \leq \theta \leq 1$

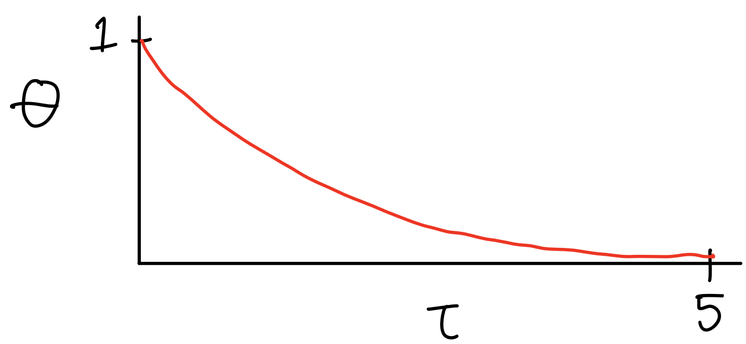
will include all the meaningful details



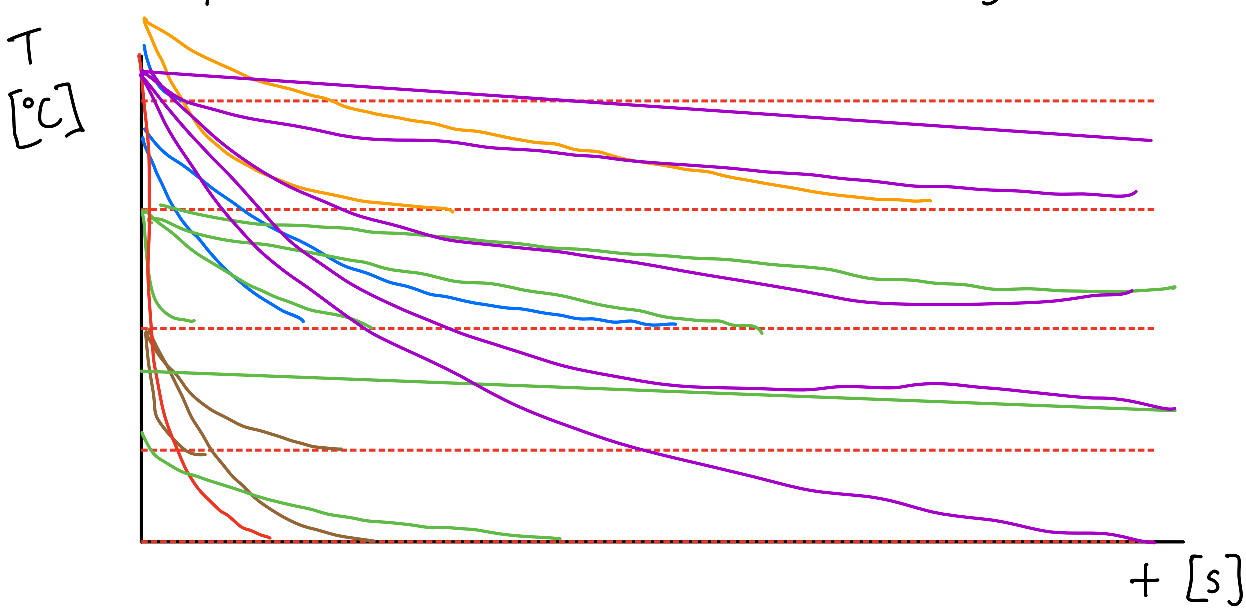
3) It is <u>always</u> a good idea to include clear, understandable figures in your technical reports.

This is arguably one of the most important ingredients to career success, and our department does not spend a lot of time teaching this!

You just have to pick it up in bits and pieces. I think a plot like this



conveys a much clearer understanding than



especially if there is a narrative accompanying it to explain how to extrapolate the result to other situations. The second plot is a trainwreck with no clear guidance on how the data is useful!