Optimization: what's the "best"?

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Due due due due due...

- Wed (Today): Pre-lecture 6.2
- Thu (Tomorrow): Assignment 5
- Fri: OSH 3 (Start early!)

For next week

Familiarize yourself with spreadsheet if you feel not comfortable enough (spreadsheet resources link)

Supporting materials for computational WeBWorK problems

Here are some videos, interactive tools and screenshots demonstrating techniques and ideas that will be useful for doing the con The first three screencasts below are difficult to see on youtube due to compression. Until they are replaced with better quality ve

The		
How to plot the graph of a function (Excel)	youtube 🚱	mov 🛃
How to zoom in and out on a graph of a function (Excel)	youtube 🗗	mov 🛃
How to add a second graph to a plot (Excel)	youtube 🗗	mov 🛃
Newton's method for solving f(x)=0 (Excel)	png	
An example of Newton's method using Google sheet	Google sheet 🙆	
	s) app 🗗	youtube 🗗
How to find the location of minimum slope for a given function (Google Sheets)	new video 🛃 (old video 삶)	
How to estimate slope using slope of secant line (Google Sheets)	youtube 🔗	
Fitting a line to data (part 1 - $y = ax$)	youtube 🗗	-
Fitting a line to data (part 2 - $y = ax + b$)	youtube 🗗	
>Euler's method for solving differential equations	youtube 🗗	

Title

Last week

- Use derivatives to characterise a function more precisely
- Sketching using calculus tools

What else can we do besides sketching? \rightarrow optimization!

This week

- unconstrained optimization
- optimization with constraints

Definition (Global extrema)

- ► A global or absolute maximum of a function f(x) over some interval I is the point where the function attains its largest value on that interval.
- ► A global or absolute minmum of a function f(x) over some interval I is the point where the function attains its smallest value on that interval.
- Check CPs and interval endpoints!

A cell of age t hours has a probability¹ of dividing given by the function

$$P(t) = \frac{at}{t^3 + 16},$$

where a is the constant $\frac{9\sqrt[6]{3}}{2\pi}$. From time t = 0 to t = 10, when is the cell likeliest to divide? When is it least likely to divide?

 $^{^1\}rm Actually$ we are giving a probability distribution function... it's a little more complicated. Still, a higher value of P(t) means that the cell is more likely to reproduce.

Example: Cell division

CP:

$$P'(t) = \frac{-2a(t^3 - 8)}{(t^3 + 16)^2}$$

Let P'(t) = 0, then t = 2.

- Classify the CP:
 - When t < 2, P'(t) > 0 (notice that a > 0).
 - When t > 2, P'(t) < 0.

By FDT, P(t) achieves local maximum at t = 2.

- ► Since the function P(t) is increasing when t < 2, and decreasing when t > 2, there would be no other point which has a higher value than P(2). Therefore, P(t) reaches the global maximum at t = 2, i.e., t = 2 is the time when a cell is likeliest to divide.
- ▶ P(0) = 0 < P(10), so t = 0 is when a cell is least likely to divide.</p>

Logistic growth

- The growth rate of a population typically depends on
 - the size of the population
 - how crowded it is
- ► The logistic growth law assumes that the growth rate of the population *G* is a function of the population density *N*:

$$G(N) = rN\left(1 - \frac{N}{K}\right)$$

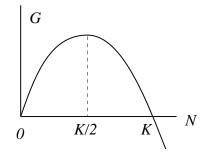
- r > 0: intrinsic growth rate
- ► K > 0: carrying capacity
- Question: what population density leads to the maximum population growth rate?

$$G(N) = rN\left(1 - \frac{N}{K}\right)$$

Q1. Sketch G as a function of N, with $N\geq 0.$ Be sure to

- 1. Identify the zeros
- 2. Find any critical points and classify them (local max/min)
- 3. Find any inflection points

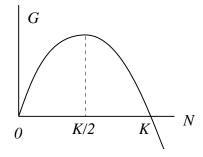
Logistic growth



▶ Zeros:
$$N = 0, K$$

▶ $G'(N) = r - \frac{2rN}{K}$, so $N = \frac{K}{2}$ is the only CP
▶ $G''(N) = -2\frac{r}{K} < 0$ so G is concave down
▶ $N = \frac{K}{2}$ is a local max

Logistic growth



- What does G(N) < 0 mean?
- Give an interpretation of the constant K.
- What population density N achieves maximum growth rate?
 - The function is first increasing and then decreasing.
 - The function is always concave down.



(Au S, Panté N. Nuclear transport of baculovirus: revealing the nuclear pore complex passage. *J Struct Biol.* 2012 Jan;177(1):90-8.)

- Baculoviruses are viruses of a cylindrical shape.
- ▶ The virus shown in this TEM image is about 800 nm long.

- Baculovirus must transport a fixed volume, K, of viral DNA and protein into an uninfected cell's nucleus.
- To maximize virus production within infected cells, a minimal amount of material is to be used to construct the membrane of the baculovirus.
- Assuming that the baculovirus has a cylindrical shape, what is the minimal surface area of the virus, given that the virus' volume must be K?

Surface area of cylinder (objective function):



There are two unknown variables r and L. What should we do?

▶ Volume of cylinder must be *K* (constraint):

$$K = \pi r^2 L$$

Re-write

$$L = \frac{K}{\pi r^2}$$

r and L are dependent! We can eliminate one.

Rewrite the constraint:

$$K = \pi r^2 L \Rightarrow L = \frac{K}{\pi r^2}$$

• Rewrite the surface area as a function of only *r*:

$$S = 2\pi r L + 2\pi r^2$$
$$S(r) = 2\frac{K}{r} + 2\pi r^2$$

Now our problem is to find the minimum value of

$$S(r) = 2\frac{K}{r} + 2\pi r^2.$$

Look for CPs:

$$S'(r) = -2\frac{K}{r^2} + 4\pi r = 0$$
$$\Rightarrow 2\frac{K}{r^2} = 4\pi r \Rightarrow r^3 = \frac{K}{2\pi} \Rightarrow r = \left(\frac{K}{2\pi}\right)^{\frac{1}{3}}$$

- Is our CP a local max or min?
- Calculate the second derivative:

$$S''(r) = 4\frac{K}{r^3} + 4\pi > 0$$

so any CP is automatically a minimum (by the Second Derivative Test).

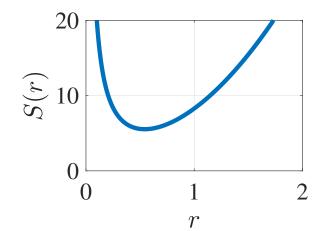
To sketch

$$S(r) = 2\frac{K}{r} + 2\pi r^2,$$

note that

- there is *one* local minima at $r = \left(\frac{K}{2\pi}\right)^{\frac{1}{3}}$
- ▶ the second derivative, S''(r) > 0, so S(r) is concave up
- For $r \ll 1$, $S(r) \approx 2\frac{K}{r}$.
- For $r \gg 1$, $S(r) \approx 2\pi r^2$.
- We're only worried about positive radius (r > 0).

Baculovirus Sketch (with K = 1)



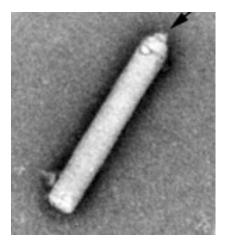
• $r = \left(\frac{K}{2\pi}\right)^{\frac{1}{3}}$ is the radius of the cylinder that has minimal surface area with volume K.

What's the length? Use the constraint!

$$K = \pi r^2 L \Rightarrow L = \frac{K}{\pi r^2}$$

► Using $r = \left(\frac{K}{2\pi}\right)^{\frac{1}{3}}$, we find the length of the cylinder is $L = \left(\frac{4K}{3}\right)^{\frac{1}{3}}$

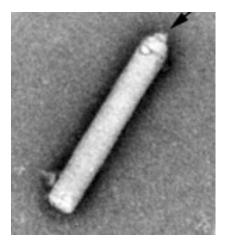
$$L = \left(\frac{4K}{\pi}\right)^{\overline{3}}.$$



 Based on our previous results, the cylinder with volume K and minimal surface area has

$$\frac{L}{r} = 2.$$

Is that true for Baculovirus?



► For Baculovirus,

$$\frac{L}{r} \neq 2.$$

 Baculovirus likely evolved other structures to be long and skinny so it can efficiently enter the nucleus though the nuclear pore complex.

- Global extrema: check the end points of an interval!
 - Cell division
- Unconstrained optimization: logistic growth
- Constrained optimization: Baculovirus
 - Use the constraints to eliminate extra dependent variables from the objective function

Find the absolute maximum of the function $f(x) = x + \frac{1}{x}$ on the interval $0.1 \le x \le 2$.