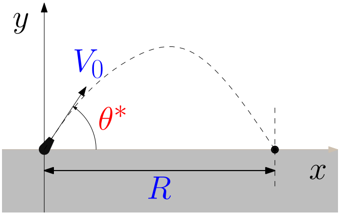
2072U Computational Science I
Winter 2022

Week	Topic
1	Introduction
1–2	Solving nonlinear equations in one variable
3–4	Solving systems of (non)linear equations
5–6	Computational complexity
6–8	Interpolation and least squares
8–10	Integration & differentiation
10–12	Additional Topics

1. Root finding: introduction
2. Iterative methods
3. First method: bisection

Example 1: hitting a target with a cannon.

To what elevation should the cannon be raised to hit the target?



Parameters:

- g = gravitational acceleration (ms^{-2}): known;
- V_0 = initial speed (ms^{-1}): known;
- R = distance to target (m): known;
- θ^* = required elevation (radians): unknown.

Determine elevation θ^* needed to hit target using known values of parameters V_0, R, and g.

- Coordinates of cannonball at time t are $(x(t), y(t))$.
- Motion of cannonball determined by Newton's 2nd law:

$$\begin{cases} x''(t) = 0, & x(0) = 0, x'(0) = V_0 \cos\theta^* \\ y''(t) = -g, & y(0) = 0, y'(0) = V_0 \sin\theta^* \end{cases}$$

- The solution to these differential equations is

$$x(t) = (V_0 \cos\theta^*)\, t$$
$$y(t) = (V_0 \sin\theta^*)\, t - \frac{1}{2} g t^2$$

- Want to find θ^* such that $x(T) = R$ and $y(T) = 0$, where T is time of flight
- Can eliminate T using $y(T) = 0$ (i.e. object is on the ground)
- If $y(T) = 0$, then $T = 0$ or $T = \dfrac{2V_0 \sin\theta^*}{g}$
- Reject $T = 0$, so to have $x(T) = R$, we must have

$$x(T) = (V_0 \cos\theta^*)\left(\frac{2V_0 \sin\theta^*}{g}\right) = R$$

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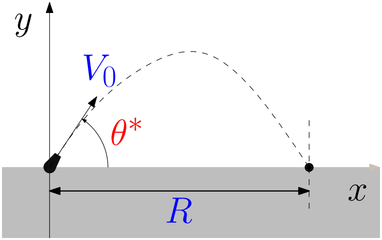
$\Rightarrow$ Zero-finding problem: find elevation θ^* such that $f(\theta^*) = 0$, where

$$f(\theta) := 2\sin\theta\cos\theta - \frac{Rg}{{V_0}^2}$$



$$f(\theta^*) = 2\sin\theta^*\cos\theta^* - \frac{Rg}{{V_0}^2}$$
$$= 0$$

We can solve this problem analytically:

- There is a unique solution $0 < \theta^* < \pi/2$ if

$$\frac{Rg}{{V_0}^2} < 1$$

- Analytic formula for θ^*:

$$\theta^* = \frac{1}{2}\arcsin\left(\frac{Rg}{{V_0}^2}\right)$$

(uses $2\sin\theta\cos\theta = \sin(2\theta)$)

In reality, there is air friction, and the equations of motion are:

$$\begin{cases} x''(t) = -c\,(x')^2, & x(0)=0,\, x'(0) = V_0 \cos\theta^* \\ y''(t) = -g - c\,y'|y'|, & y(0)=0,\, y'(0) = V_0 \sin\theta^* \end{cases}$$

$$x(t) = \frac{1}{c}\ln\left(c\,V_0\,t\cos\theta^* + 1\right)$$

$$y(t) = \begin{cases} \frac{1}{c}\ln\left(\cos(\sqrt{cg}\,t) + \sin(\sqrt{cg}\,t)\sqrt{\frac{c}{g}}\,V_0\sin\theta^*\right) & \text{for } t \le t' \\ -\frac{1}{c}\ln\left(\cosh(\sqrt{cg}[t-t'])\right) \\ \qquad -\frac{1}{c}\ln\left(\cos(\arctan(\sqrt{\frac{c}{g}}\,V_0\sin\theta^*))\right) & \text{for } t > t' \end{cases}$$

where

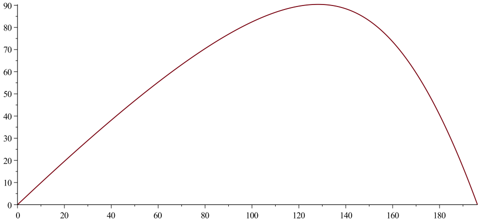
$$t' = \frac{1}{\sqrt{cg}}\arctan\left(\sqrt{\frac{c}{g}}\,V_0\sin\theta^*\right)$$

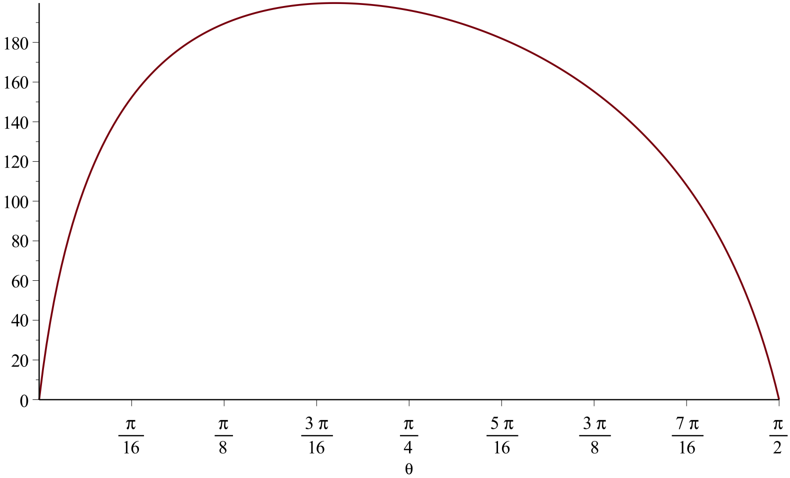
is the time at which the ball is at its highest point ($y'(t') = 0$).

1. Solve for t^* from $y(t^*) = 0$.
2. Find the distance of impact as $x(t^*)$:

$$x(t^*) = \frac{1}{c} \ln \left[\sqrt{\frac{c}{g}} V_0 \cos \theta^* \left(\arctan \left[\sqrt{\frac{c}{g}} V_0 \sin \theta^* \right] + \operatorname{arccosh} \left[\sqrt{\frac{g + c V_0^2 \sin^2 \theta^*}{g}} \right] \right) + 1 \right]$$

3. Solve for θ^* from $x(t^*) = R$...

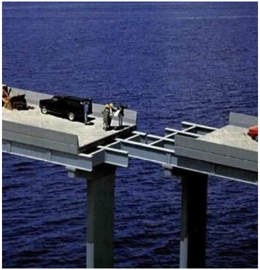



180
160
140
120
100
80
60
40
20
0
$\frac{\pi}{16}$
$\frac{\pi}{8}$
$\frac{3\pi}{16}$
$\frac{\pi}{4}$
$\frac{5\pi}{16}$
$\frac{3\pi}{8}$
$\frac{7\pi}{16}$
$\frac{\pi}{2}$
θ

We cannot find an analytic solution anymore.
Instead, we must look for a numerical approximation like

$$\theta^* = 0.19 \pm 10^{-2}$$

where $\Delta\theta^* = 10^{-2}$ is the *absolute error*.
This error needs to be small enough for the application.

Example 2: pension payments

Suppose you pay an amount of money to a bank every year and they promise to pay you a lump sum when you retire. Over one year, you would pay an amount

$$\nu P = \frac{1}{1+i} P \quad (i \text{ is the percentage interest rate})$$

for this service to compensate fo the loss of interest.
Over n years you will pay

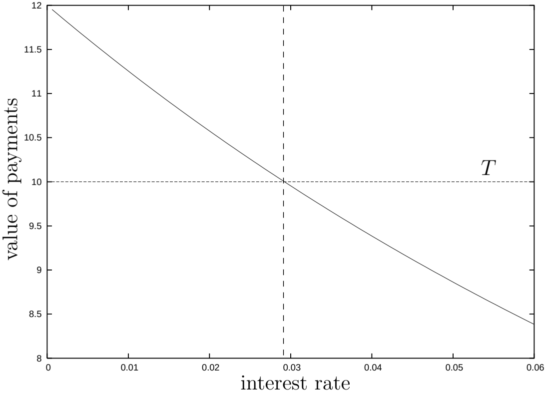
$$\nu P + \nu^2 P + \ldots + \nu^n P = \nu P \frac{1-\nu^n}{1-\nu} = T$$

for a lump sum payment of nP.

Now suppose we *know* the total value and *want to know* the interest rate. We then have to solve the following equation:

$$\nu \frac{1-\nu^n}{1-\nu} = \frac{1}{i} - \frac{1}{i}\left(\frac{1}{1+i}\right)^n = T/P$$

For example, let $n = 12$, $T/P = 10$.



In order to find the interest rate i^* we must solve a nonlinear equation

$$f(i) = \frac{1}{i} - \frac{1}{i}\left(\frac{1}{1+i}\right)^n - T/P = 0$$

to find an answer like

$$i^* = 0.0292285 \pm 2 \times 10^{-7}$$

For this end,we can use *iterative* methods.
The two methods we will study here are

1. *bisection*
2. *Newton's method* (and an adaptation called the *secant method*).

Iterative methods

- Algorithms for solving $f(x^*) = 0$ are usually iterative.
- Starting from $x^{(0)}$, make sequence of iterates

$$
\begin{aligned}
x^{(1)} &= \phi\left(x^{(0)}\right), \\
x^{(2)} &= \phi\left(x^{(1)}\right), \\
&\vdots \\
x^{(k+1)} &= \phi\left(x^{(k)}\right), \\
&\vdots
\end{aligned}
$$

  ϕ function/rule generating successive iterates
- Rule $x^{(k+1)} = \phi\left(x^{(k)}\right)$ for $k \geq 0$ is recurrence relation.

Simple example

$x^{(0)} := 1$ and $\phi : \mathbb{R} \to \mathbb{R}$ is the function given by

$$(\forall t \in \mathbb{R}) \qquad \phi(t) = 2t$$

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$$x^{(0)} = 1$$
$$x^{(1)} = 2 \cdot x^{(0)} = 2 \cdot 1 = 2$$

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$$\begin{aligned} x^{(0)} &= 1 \\ x^{(1)} &= 2 \cdot x^{(0)} = 2 \cdot 1 = 2 \\ x^{(2)} &= 2 \cdot x^{(1)} = 2 \cdot 2 = 4 \end{aligned}$$

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x^{(3)} &= 2 \cdot x^{(2)} = 2 \cdot 4 = 8
\end{aligned}$$

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x^{(0)} &= 1 \\
x^{(1)} &= 2 \cdot x^{(0)} = 2 \cdot 1 = 2 \\
x^{(2)} &= 2 \cdot x^{(1)} = 2 \cdot 2 = 4 \\
x^{(3)} &= 2 \cdot x^{(2)} = 2 \cdot 4 = 8 \\
x^{(4)} &= 2 \cdot x^{(3)} = 2 \cdot 8 = 16 \\
&\vdots \\
x^{(k)} &= 2^k
\end{aligned}$$

k	$x^{(k)}$
0	1
1	2
2	4
3	8
4	16
$\vdots$	$\vdots$
k	2^k

Less simple example

- Given $a > 0$ and $x^{(0)} > 0$, consider sequence

$$x^{(k+1)} = \phi\left(x^{(k)}\right) = \frac{1}{2}\left(x^{(k)} + \frac{a}{x^{(k)}}\right) \qquad (k = 0, 1, \ldots)$$

k	$x^{(k)}$
0	3.00000000000000
1	
2	
3	
4	
5	

This sequence converges to $\sqrt{5}$!

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$$x^{(k+1)} = \phi\left(x^{(k)}\right) = \frac{1}{2}\left(x^{(k)} + \frac{a}{x^{(k)}}\right) \qquad (k = 0, 1, \dots)$$

- e.g., with $a = 5$ and $x^{(0)} = 3$, we get

k	$x^{(k)}$
0	3.00000000000000
1	
2	
3	
4	
5	

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k	$x^{(k)}$
0	3.00000000000000
1	2.33333333333333
2	
3	
4	
5	

This sequence converges to $\sqrt{5}$!

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1	2.33333333333333
2	2.23809523809524
3	
4	
5	

This sequence converges to $\sqrt{5}$!

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0	3.00000000000000
1	2.33333333333333
2	2.23809523809524
3	2.23606889564336
4	
5	

This sequence converges to $\sqrt{5}$!

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0	3.00000000000000
1	2.33333333333333
2	2.23809523809524
3	2.23606889564336
4	2.23606797749998
5	

This sequence converges to $\sqrt{5}$!

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- e.g., with $a = 5$ and $x^{(0)} = 3$, we get

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0	3.00000000000000
1	2.33333333333333
2	2.23809523809524
3	2.23606889564336
4	2.23606797749998
5	2.23606797749979

This sequence converges to $\sqrt{5}$!

- Circa 1800-1600 BCE
- Numbers on diagonal

$$1;24;51;10 = 1 + \frac{24}{60^1} + \frac{51}{60^2} + \frac{10}{60^3}$$
$$\simeq \sqrt{2} \text{ to 9 decimal places!}$$

- Tablet suggests Babylonians knew Pythagoras's theorem

$$a^2 + b^2 = c^2$$

relating sides of right-angled triangle

Convergence of iterations

- Any iteration $x^{(k+1)} = \phi(x^{(k)})$ generates a sequence

$$\left\{x^{(k)}\right\}_{k=0}^{\infty} = \left\{x^{(0)}, x^{(1)}, x^{(2)}, \ldots, x^{(k-1)}, x^{(k)}, x^{(k+1)}, \ldots\right\}$$

- Recall: limit of sequence $\left\{x^{(k)}\right\}_{k=0}^{\infty}$ is $x^* \in \mathbb{R}$ iff

$$(\forall \epsilon > 0)(\exists K \in \mathbb{N}) \; \left[(k \geq K) \Rightarrow \left|x^{(k)} - x^*\right| < \epsilon\right]$$

- In words, the sequence $\left\{x^{(k)}\right\}_{k=0}^{\infty}$ converges to $x^* \in \mathbb{R}$ or

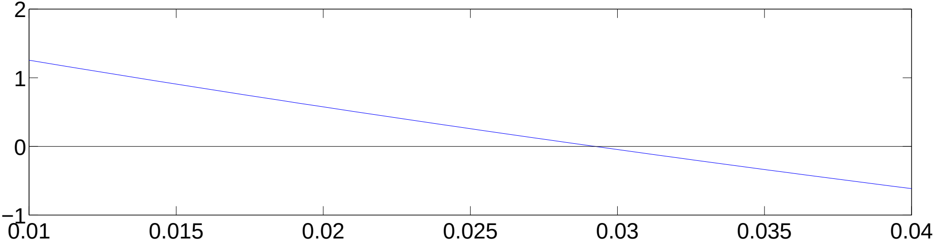
$$\boxed{\lim_{k\to\infty} x^{(k)} = x^*}$$

Bisection

Suppose we have a continuous function f on some domain $[a, b]$, and that there is a unique solution

$$f(x^*) = 0, \quad x^* \in [a, b]$$

then $f(a)f(b) < 0$. Example:



Or, in *pseudo-code*:

Input: f, a, b, $k_{\max}$, ϵ_x, ϵ_f.

1. Set $a_0 = a$, $b_0 = b$.
2. Do for $k = 1, \ldots, k_{\max}$
   - Let $c_k = (a_{k-1} + b_{k-1})/2$ and $f_k = f(c_k)$.
   - If $f_k f(a_{k-1}) > 0$ then let $a_k = c_k$ and $b_k = b_{k-1}$ else let $a_k = a_{k-1}$ and $b_k = c_k$.
   - If $|b_k - a_k| < \epsilon_x$ or $|f(c_k)| < \epsilon_f$ break.
3. Return $x^* = c_k$ and $|b_k - a_k|$.