Scientific Computing – Primary Purpose of Computers

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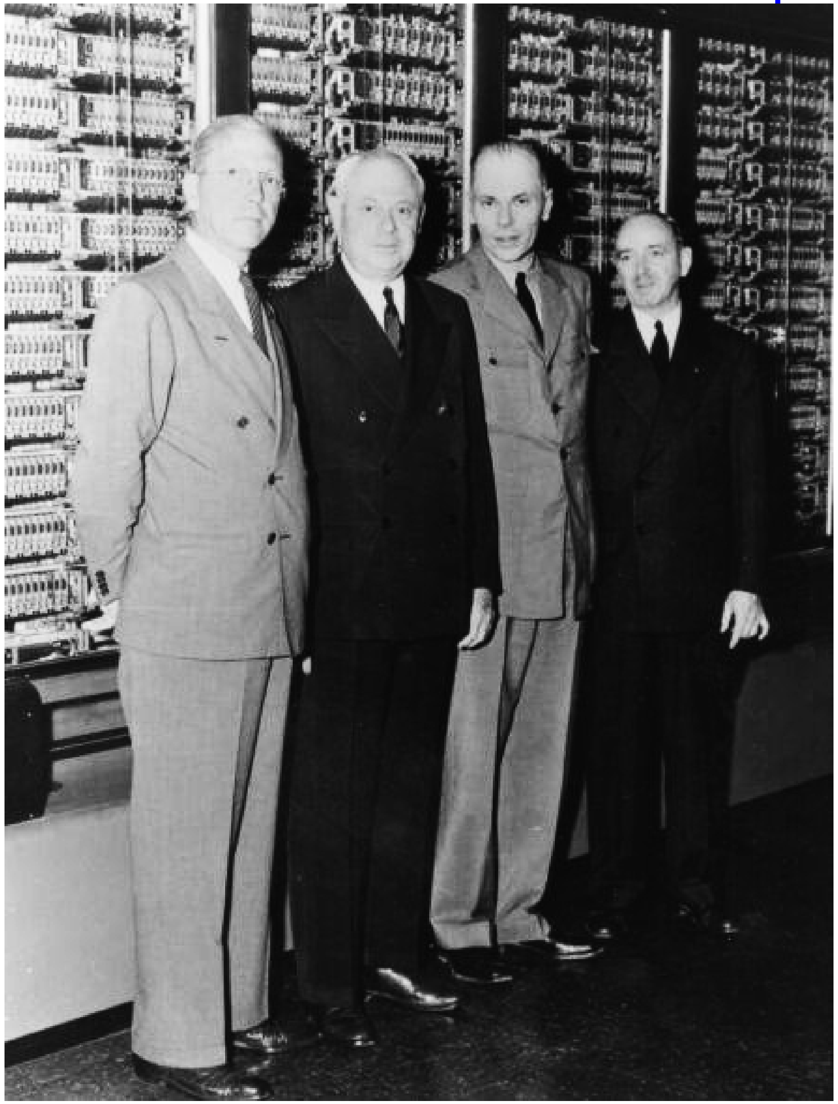
Some Computer History

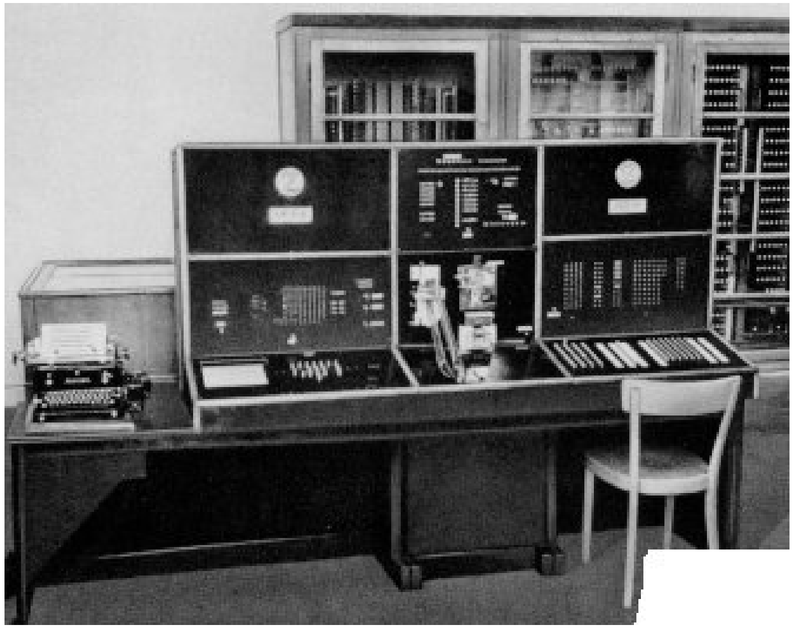


Howard Aiken, second right

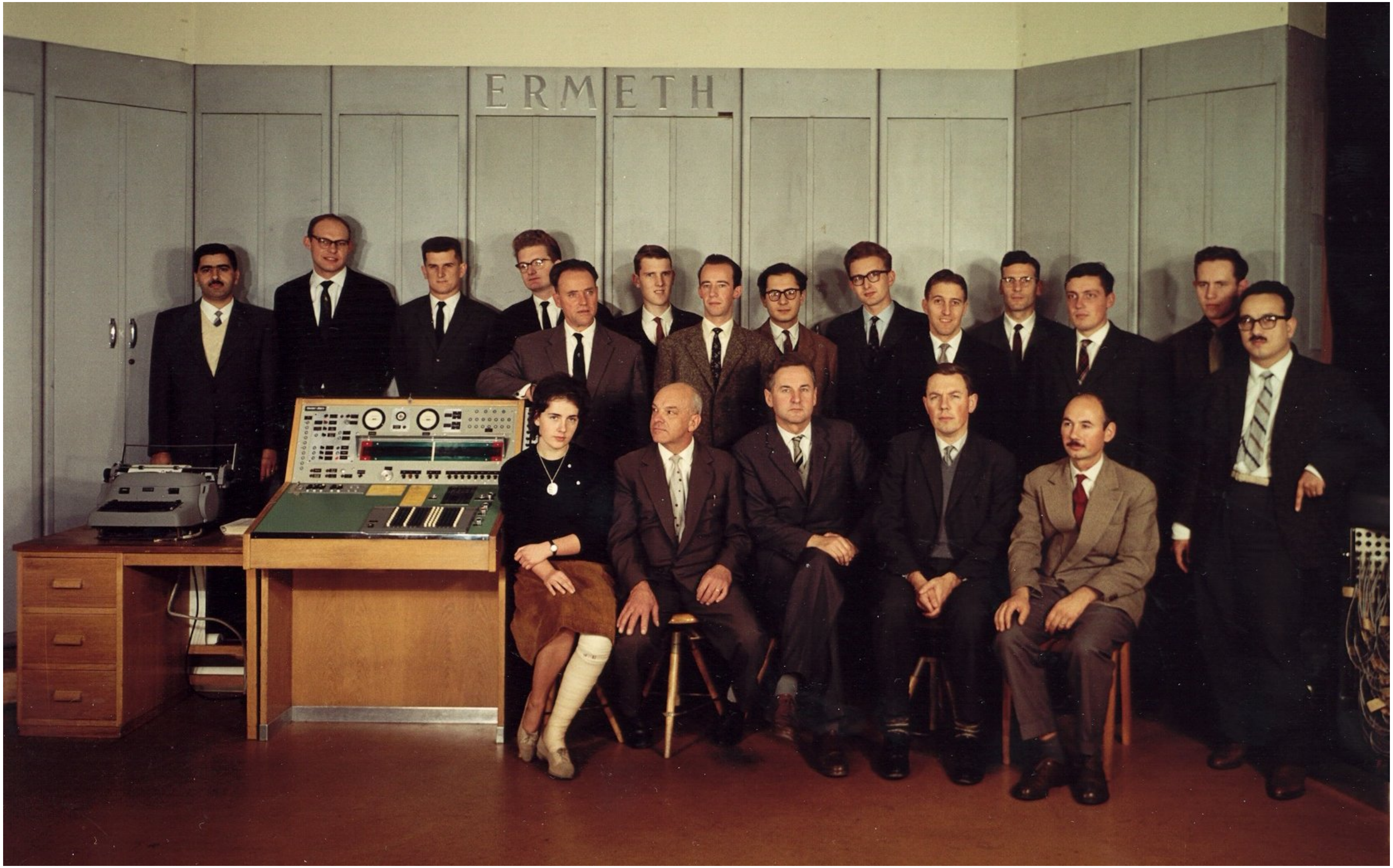
Konrad Zuse

Zuse's Z4 at ETH (1950-1955)

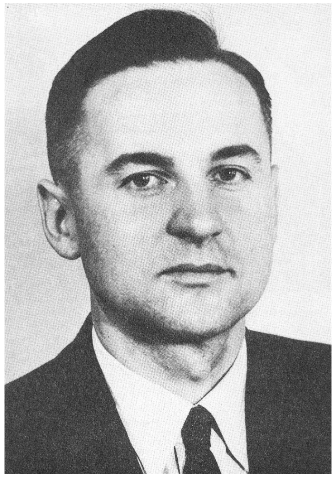
A. Speiser, H. Rutishauser (1955)



Prof. Stiefel and his collaborators in front of Z4

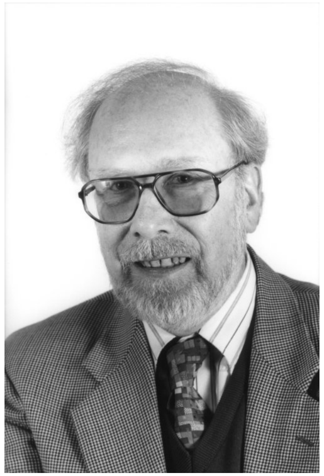

ERMETH

Developer of Programming Languages



One of the fathers of ALGOL

Handbook Series Vol 1:
HEINZ RUTISHAUSER
Description of ALGOL 60
Springer 1967



PASCAL: Report by KATHLEEN JENSEN and NIKLAUS WIRTH, 1975

MODULA: Programming in Modula-2 by NIKLAUS WIRTH, 1982

OBERON: J. GUTKNECHT, N. WIRTH: Project Oberon. The Design of an Operating System and Compiler, 1992

1991 Fred Brooks, Chairman W. Gander, Konrad Zuse

Computer today

- writing with text processor
- surfing, search for information on the WEB
- communication: Chatting/e-mail/Skype/Bloggs via Internet
- store music, copy
- view movies, DVD
- computer games
- store and process photos

But in effect

Computer

What has to be computed?

The World of Computers is Digital

- All data are binary coded numbers
- continuous signals have to be discretized (= represented by a finite set of numbers) to be processed on a computer
- a computer understands/processes/stores only numbers
- when processing the data (=binary coded numbers) the computer has to

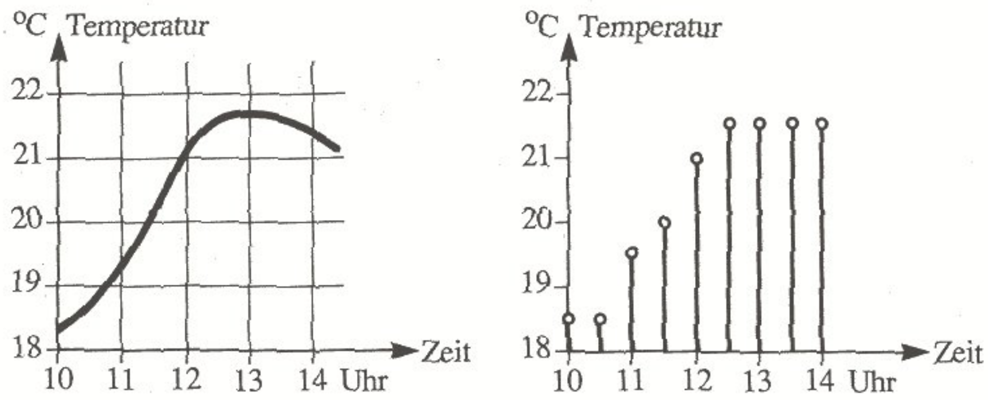
compute!

Every character is binary coded

ASCII Code (section) (has been enlarged and replaced by UNICODE Standard)

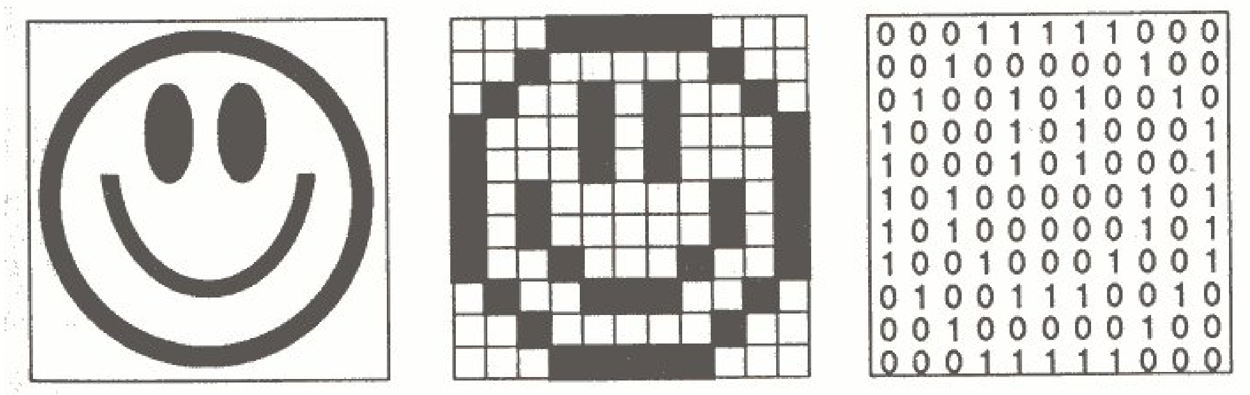
character	decimal	hex	binary	character	decimal	hex	binary
a	97	61	01100001	0	48	30	00110000
b	98	62	01100010	1	49	31	00110001
c	99	63	01100011	2	50	32	00110010
d	100	64	01100100	3	51	33	00110011
e	101	65	01100101	4	52	34	00110100
f	102	66	01100110	5	53	35	00110101
g	103	67	01100111	6	54	36	00110110
h	104	68	01101000	7	55	37	00110111
i	105	69	01101001	8	56	38	00111000
j	106	6A	01101010	9	57	39	00111001

- Analog – Discrete – Digitized



10.00	18.5
10.30	18.5
11.00	19.5
11.30	20.0
12.00	21.0
12.30	21.5
13.00	21.5
13.30	21.5
14.00	21.5

- pictures: discretized and digitized



- Compact Disk: sound pressure 44'100 samplings/Sec, $2^{16} = 65'536$ states

Scientific Computing

= Primary Purpose of Computers:

compute numerical approximations to solutions of equations when analytical solutions don't exist or when computational effort too large

- Konrad Zuse:
  solve large (back then $n = 20$) systems of linear equations
  Today: my collaborator Peter Arbenz at ETH solved systems of linear equations with billions ($n = 10^9 = 1'000'000'000$) of unknowns

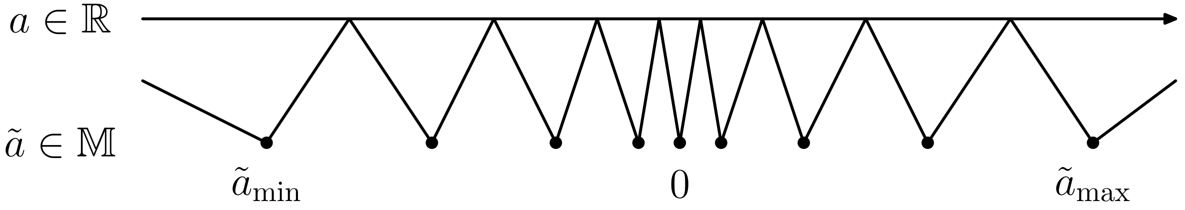
- Howard Aiken:
  system of differential equations with several functions, no analytic solution thus needs to compute numerical solutions

How does a computer performs computations with real numbers?

Number Representation in a Computer

real numbers $\leftrightarrow$ machine numbers

- mathematics: real numbers $\mathbb{R}$ = continuum
  every interval $(a, b) \in \mathbb{R}$ with $a < b$ contains ∞ set of numbers
- computer: finite machine, can only
  - store a finite set of numbers
  - perform a finite number of operations
- computer: the machine numbers $\mathbb{M}$ (finite set)
- mapping $\mathbb{R} \to \mathbb{M}$: a whole interval $\in \mathbb{R} \to \tilde{a} \in \mathbb{M}$:



computer calculate on principle inaccurately!

Matlab program	results
$a = 10$	$a = 10$
$b = a/7$	$b = 1.428571428571429$
$c = sqrt(sqrt(sqrt(sqrt(b))))$	$c = 1.022542511383932$
$d = exp(16 * log(c))$	$d = 1.428571428571427$
$e = d * 7$	$e = 9.999999999999991$
$a - e$	$ans = 8.881784197001252e{-}15$

real numbers in computer: decimal numbers of about 16 digit (IEEE Floating Point Standard)

study/controlling of rounding errors $\Rightarrow$ numerical analysis

IEEE Floating Point Standard (since 1985)

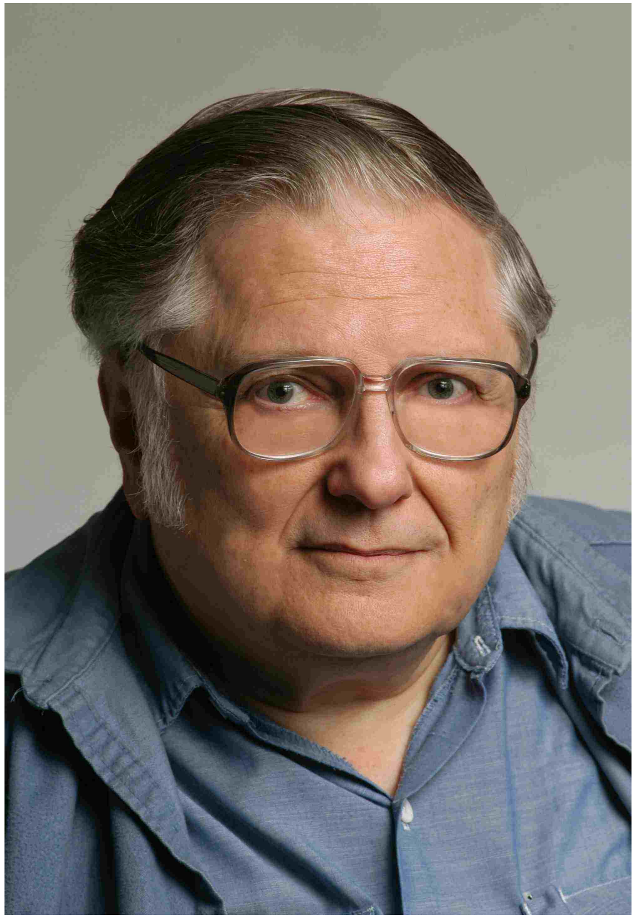
- a real number is represented as floating point number using 64 bits

$$\underset{0}{S} \quad \overbrace{\underset{1}{E}EEEEEEEEE\underset{11}{E}}^{e} \quad \overbrace{\underset{12}{F}FFFF\cdots FFFF\underset{63}{F}}^{m}$$

- normal case: $0 < e < 2047, \quad (2^{11} = 2048)$

$$\tilde{a} = (-1)^S \times 2^{e-1023} \times 1.m$$

- realmin $= 2.2251 \cdot 10^{-308} = 2^{-1022}$
  realmax $= 1.7977 \cdot 10^{308}$
- underflow, overflow



William Kahan
(Father IEEE F.P.S.)

correct program – results nevertheless wrong!

compute π as limit of regular polygons with n edges

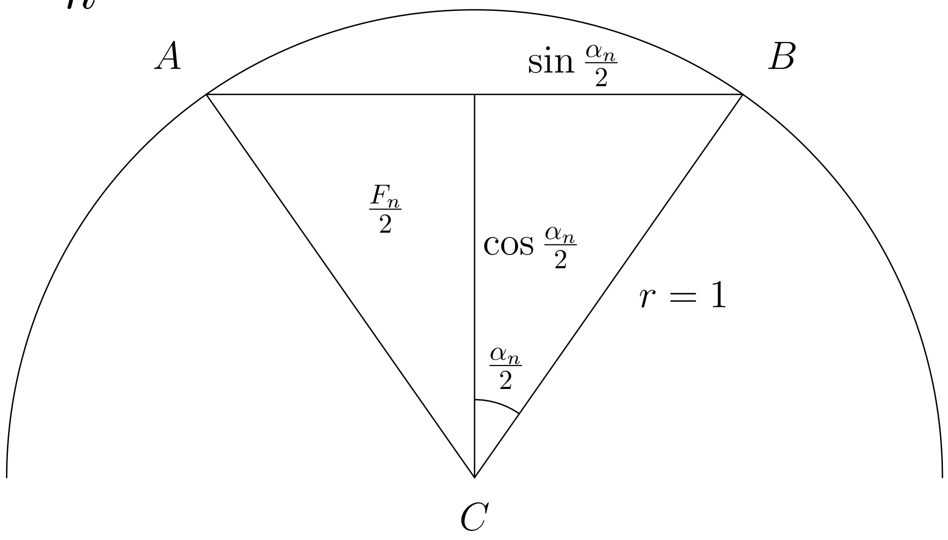
- A_n: area of the n-polygon

$$A_n = n\,F_n = \frac{n}{2}\sin\alpha_n, \quad \alpha_n = \frac{2\pi}{n}$$

- $\lim_{n\to\infty} A_n = \pi$
- $A_6 = \frac{3}{2}\sqrt{3} = 2.5981$
  $A_{12} = 3$
- recursion $A_n \to A_{2n}$

$$\sin\left(\frac{\alpha}{2}\right) = \sqrt{\frac{1-\sqrt{1-\sin^2\alpha}}{2}}$$

only 2 square roots and rational operations



program

pinaive

```
s=sqrt(3)/2; A=3*s; n=6;            % initialization
z=[A-pi n A s];                     % store the results
while s>1e-10                       % termination if s=sin(alpha) small
  s=sqrt((1-sqrt(1-s*s))/2);        % new sin(alpha/2) value
  n=2*n; A=n/2*s;                   % A = new polygon area
  z=[z; A-pi n A s];
end
m=length(z);
for i=1:m
  fprintf('%10d %20.15f %20.15f %20.15f\n',z(i,2),z(i,3),z(i,1),z(i,4))
end
```

Stabilizing by rewriting algebraically avoiding cancellation

$$\sin\frac{\alpha_n}{2} = \sqrt{\frac{1-\sqrt{1-\sin^2\alpha_n}}{2}} \quad \text{unstable recursion}$$

$$= \sqrt{\frac{1-\sqrt{1-\sin^2\alpha_n}}{2}\,\frac{1+\sqrt{1-\sin^2\alpha_n}}{1+\sqrt{1-\sin^2\alpha_n}}}$$

$$= \sqrt{\frac{1-(1-\sin^2\alpha_n)}{2(1+\sqrt{1-\sin^2\alpha_n})}}$$

$$\sin\frac{\alpha_n}{2} = \frac{\sin\alpha_n}{\sqrt{2(1+\sqrt{1-\sin^2\alpha_n})}} \quad \text{stable recursion}$$

Program

pistabil

```
oldA=0;s=sqrt(3)/2; newA=3*s; n=6;      % initialization
z=[newA-pi n newA s];                   % store the results
while newA>oldA                         % quit if area does not increase
   oldA=newA;
   s=s/sqrt(2*(1+sqrt((1+s)*(1-s)))); % new sin-value
   n=2*n; newA=n/2*s;
   z=[z; newA-pi n newA s];
end
m=length(z);
for i=1:m
  fprintf('%10d %20.15f %20.15f\n',z(i,2),z(i,3),z(i,1))
end
```

nonlinear equations

$$x^2 - 5x + 6 = 0 \quad \text{oder} \quad e^x + x = 0$$

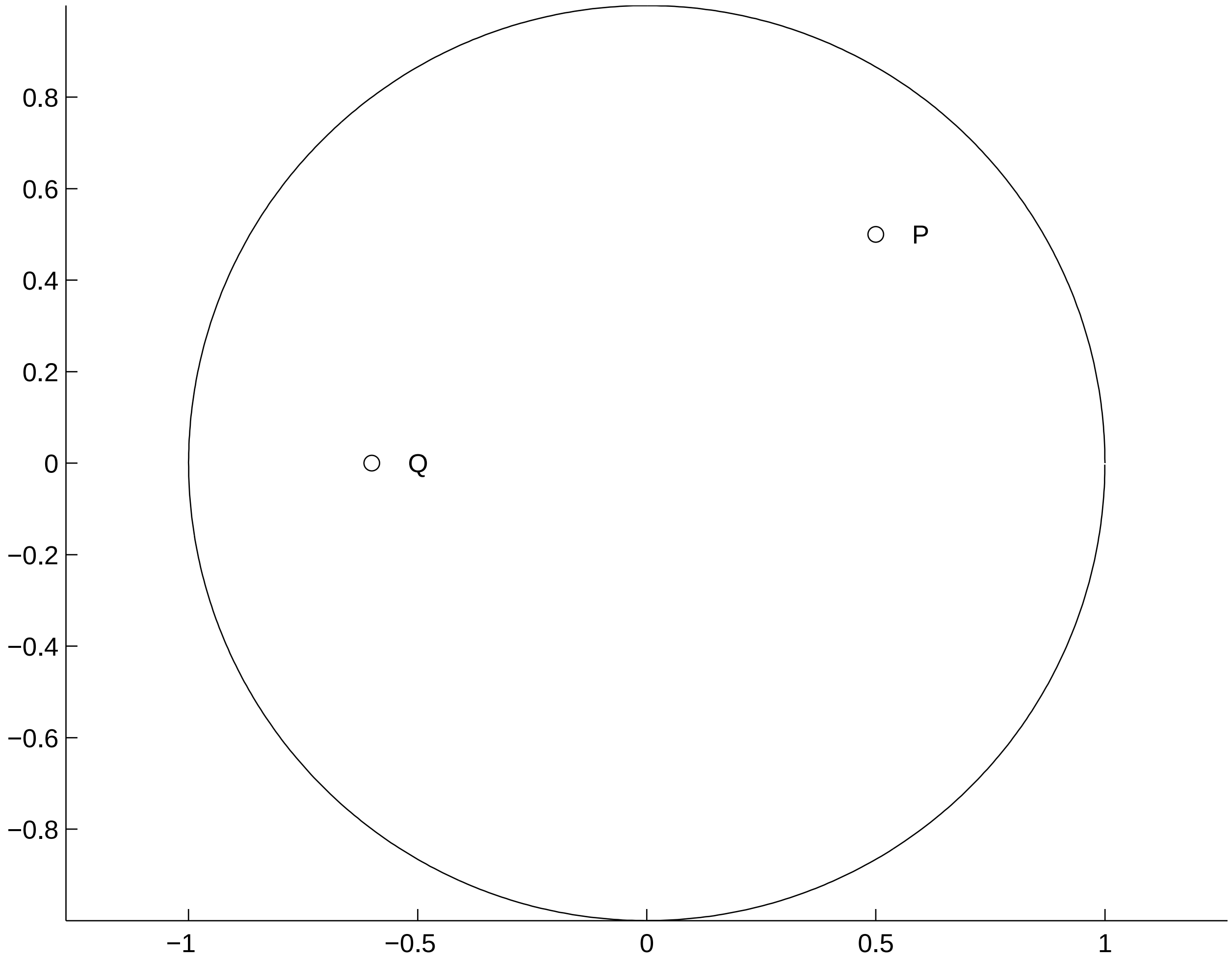
- solution: we are looking for numbers

$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \Rightarrow \quad x_1 = 2,\ x_2 = 3$$

- $e^x + x = 0$ is only solvable by a numerical approximation.
  The only solution is $x \approx -0.5671432904$:

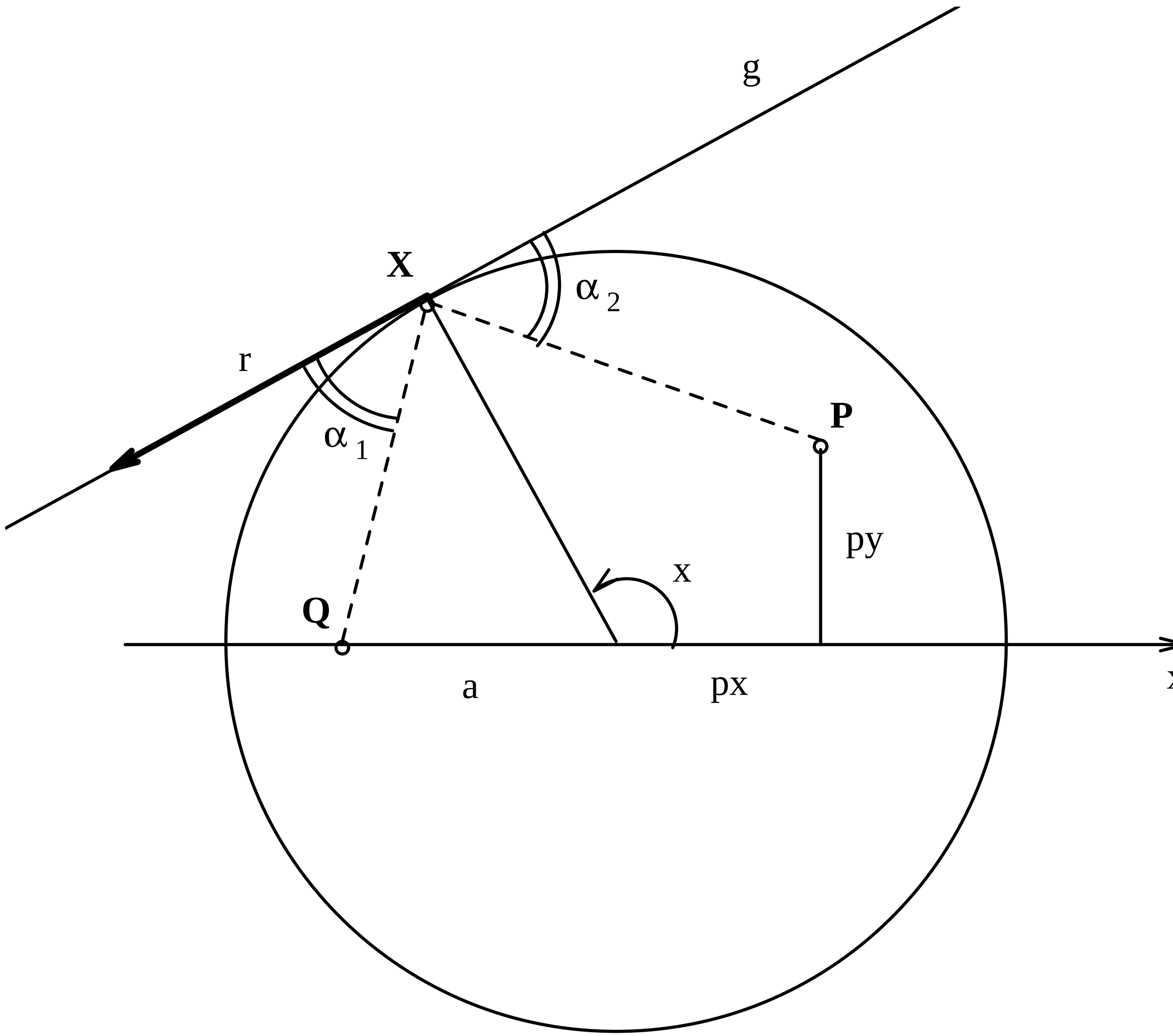
$$e^{-0.5671432904} - 0.5671432904 = 1.5333 \times 10^{-11} = 0.000000000001533$$

example for an equation: circular billiard



Modelling

- rotational symmetry wlog
  $\Rightarrow Q$ on x-axis
- circle radius
  wlog $r = 1$,
  $$\mathbf{X} = \begin{pmatrix} \cos x \\ \sin x \end{pmatrix}$$
  $$\Rightarrow \mathbf{r} = \begin{pmatrix} -\sin x \\ \cos x \end{pmatrix}$$
- Law of reflection
  $\alpha_1 = \alpha_2 \iff$
  $f(x) = (\mathbf{e}_{XQ} + \mathbf{e}_{XP})^T \mathbf{r} = 0$
  equation for x



A computer-algebra system manipulates formulas

We compute $f(x)$ with Maple

```
c   :=   cos(x);     s  := sin(x);
xp1  := px-c  ;   xp2  := py-s;
xq1  :=   a-c  ;   xq2  := -s;

h  := sqrt(xp1^2 + xp2^2);
ep1  := xp1/h;
ep2  := xp2/h;

h  := sqrt(xq1^2 + xq2^2);
eq1   := xq1/h;
eq2   := xq2/h;

f  := (ep1+eq1)*s - (ep2+eq2)*c;
```

Result of Maple computation

→ bill.mw

red: given parameters, balls $P = (px, py)$ and $Q = (a, 0)$

$$f(x) := \left(\frac{px - \cos x}{\sqrt{(px - \cos x)^2 + (py - \sin x)^2}} + \frac{a - \cos x}{\sqrt{(a - \cos x)^2 + \sin x^2}} \right) \sin x$$

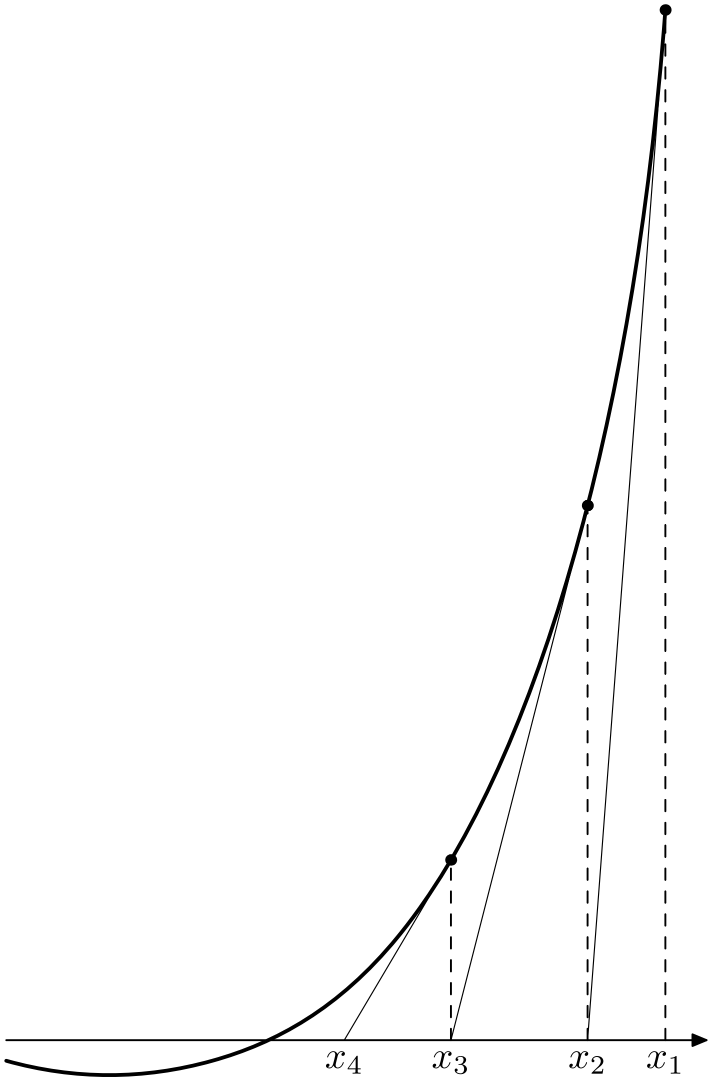
$$- \left(\frac{py - \sin x}{\sqrt{(px - \cos x)^2 + (py - \sin x)^2}} - \frac{\sin x}{\sqrt{(a - \cos x)^2 + \sin x^2}} \right) \cos x$$

we want to solve the equation $f(x) = 0$

Solution using Newton's method

- $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$

- we need the derivative of $f(x)$



Derivative $f'(x)$

A computer algebra system can compute derivatives. The Maple command `df := D(f); df(x);` delivers a complicates expression:

$$f'(x) =$$

$$\left(\frac{\sin(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} - 1/2\,\frac{(px-\cos(x))(2\,(px-\cos(x))\sin(x)-2\,(py-\sin(x))\cos(x))}{\left((px-\cos(x))^2+(py-\sin(x))^2\right)^{3/2}} + \right.$$

$$\left.\frac{\sin(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}} - 1/2\,\frac{(a-\cos(x))(2\,(a-\cos(x))\sin(x)+2\,\sin(x)\cos(x))}{\left((a-\cos(x))^2+(\sin(x))^2\right)^{3/2}}\right)\sin(x) +$$

$$\left(\frac{px-\cos(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} + \frac{a-\cos(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}}\right)\cos(x)$$

$$-\left(-\frac{\cos(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} - 1/2\,\frac{(py-\sin(x))(2\,(px-\cos(x))\sin(x)-2\,(py-\sin(x))\cos(x))}{\left((px-\cos(x))^2+(py-\sin(x))^2\right)^{3/2}} - \right.$$

$$\left.\frac{\cos(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}} + 1/2\,\frac{\sin(x)(2\,(a-\cos(x))\sin(x)+2\,\sin(x)\cos(x))}{\left((a-\cos(x))^2+(\sin(x))^2\right)^{3/2}}\right)\cos(x) +$$

$$\left(\frac{py-\sin(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} - \frac{\sin(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}}\right)\sin(x)$$

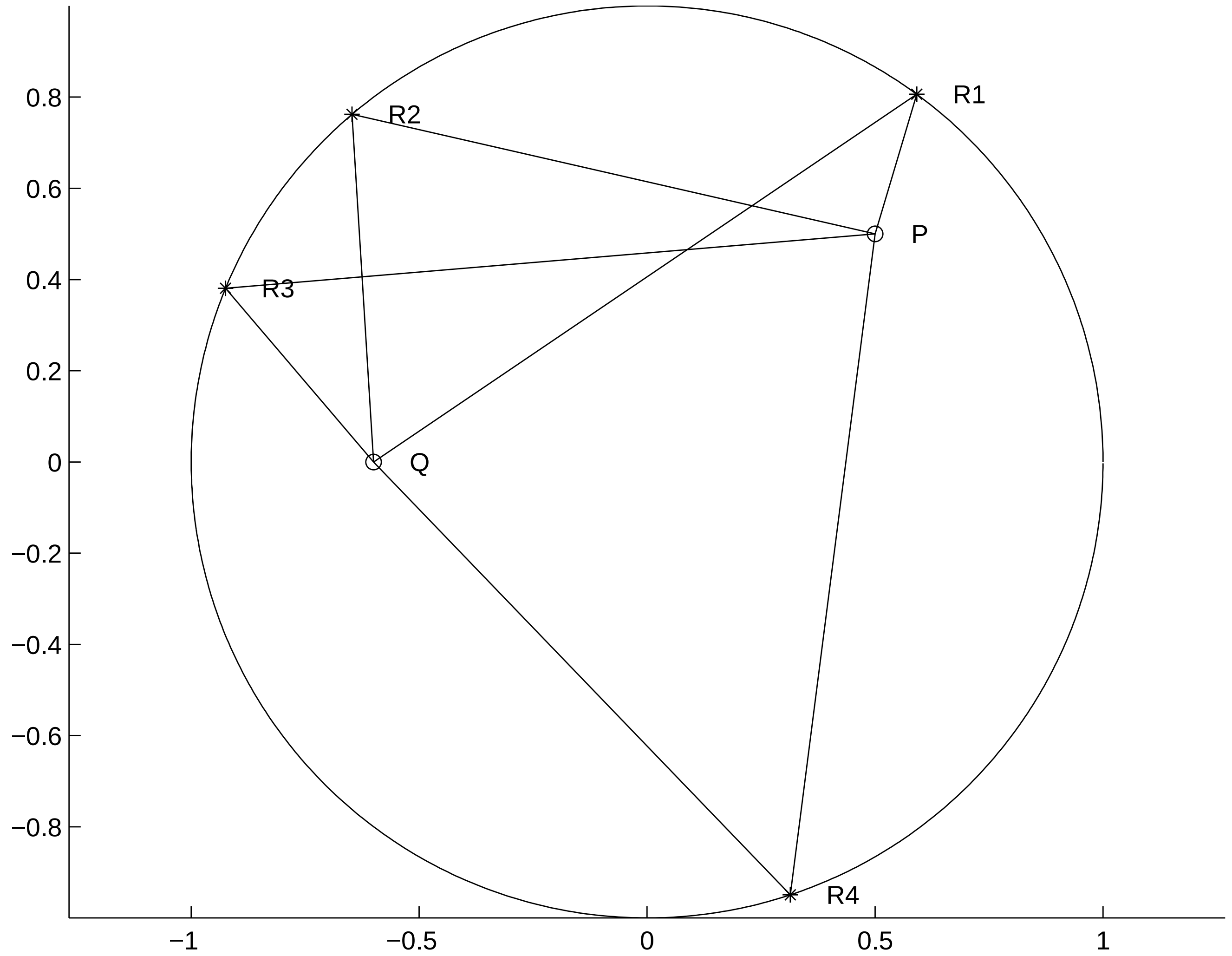
Better way using algorithmic differentiation

differentiation of programs!

```
function [y ys] = ffs(x)
% computes the functions f and its derivative  fs for the
% billiard problem
global px py a
 cs = -sin(x);                                      c =  cos(x);
 ss = cos(x);                                       s = sin(x);
 xp1s =  -cs ; xp2s =  -ss;                         xp1 = px-c ;  xp2 = py-s;
 xq1s =   -cs ; xq2s = -ss;                         xq1 =  a-c ;  xq2 = -s;
 hs = (xp1*xp1s + xp2*xp2s)/sqrt(xp1^2 + xp2^2);    h = sqrt(xp1^2 + xp2^2);
 ep1s = (h*xp1s - xp1*hs)/h^2;                      ep1 = xp1/h;
 ep2s = (h*xp2s - xp2*hs)/h^2;                      ep2 = xp2/h;
 hs = (xq1*xq1s + xq2*xq2s)/sqrt(xq1^2 + xq2^2);    h = sqrt(xq1^2 + xq2^2);
 eq1s = (h*xq1s - xq1*hs)/h^2;                      eq1  = xq1/h;
 eq2s = (h*xq2s - xq2*hs)/h^2;                      eq2  = xq2/h;
 ys = (ep1s+eq1s)*s+(ep1+eq1)*ss-(ep2s+eq2s)*c-(ep2+eq2)*cs;
                                                    y = (ep1+eq1)*s - (ep2+eq2)*c;
```

Solutions for $P = (0.5, 0.5)$ and $Q = (-0.6, 0)$ → main

We get 4 solutions using different starting values for Newton's iteration



Is there an "analytical" solution?

"Rationalizing formulas": new variable $t = \tan(x/2)$

$\Rightarrow \sin(x) = \frac{2t}{(1+t^2)}, \quad \cos(x) = \frac{1-t^2}{1+t^2}$ in $f(x)$ insert:

$$f(x) = g(t) = \frac{2\,t}{1+t^2}\left(\frac{px - \frac{1-t^2}{1+t^2}}{\sqrt{\left(px - \frac{1-t^2}{1+t^2}\right)^2 + \left(py - \frac{2\,t}{1+t^2}\right)^2}} + \frac{a - \frac{1-t^2}{1+t^2}}{\sqrt{\left(a - \frac{1-t^2}{1+t^2}\right)^2 + \frac{4\,t^2}{(1+t^2)^2}}}\right)$$

$$-\frac{1-t^2}{1+t^2}\left(\frac{py - \frac{2\,t}{1+t^2}}{\sqrt{\left(px - \frac{1-t^2}{1+t^2}\right)^2 + \left(py - \frac{2\,t}{1+t^2}\right)^2}} - \frac{2\frac{t}{1+t^2}}{\sqrt{\left(a - \frac{1-t^2}{1+t^2}\right)^2 + \frac{4\,t^2}{(1+t^2)^2}}}\right) = 0$$

Even more complicates equation! However, surprise:

```
> solve(g = 0, t);
```

$$RootOf((py\,a + py)\,\_Z^4 + (4\,px\,a + 2\,a + 2\,px)\,\_Z^3 - 6\,\_Z^2 py\,a + (-4\,px\,a + 2\,a + 2\,px)\,\_Z - py + py\,a)$$

Summary: the billiard problem shows different concepts:

- Modelling of the problem
- deriving the equation by means of a computer algebra system
- differentiation of programs, algorithmic differentiation
- “Analytical” solution by means of the rationalizing formulas furnishes the equation $(a+1)py\,t^4 + (4a\,px + 2a + 2px)\,t^3 - 6a\,py\,t^2 + (-4a\,px + 2a + 2px)\,t + (a-1)py = 0$, which proves that the problem has at most 4 solutions.
- support by computer for
  - for numerical computations
  - and for algebraic manipulations

  is very useful!

Differential Equations

- $$y'(x) = 2\,y(x)$$

  The solutions are functions

  $$y(x) = e^{2x} \quad \Rightarrow \quad y'(x) = 2\,e^{2x} = 2\,y(x)$$

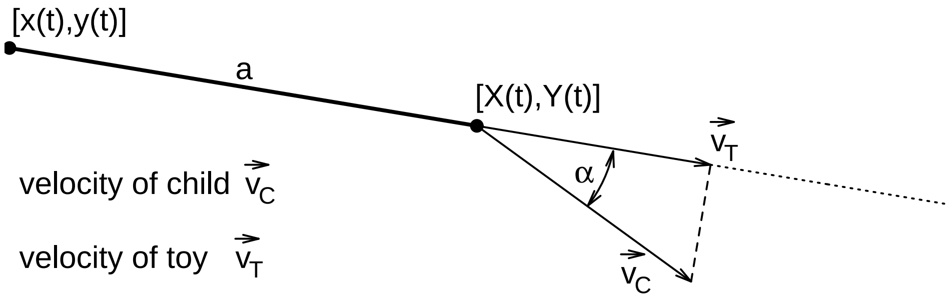
- A curve is described in parametric form e.g. an ellipse:

  $$x(t) = a\cos(t), \quad y(t) = b\sin(t), \quad 0 \leq t \leq 2\pi$$

- A differential equation which has a curve as solution is a system of two equations for the two functions $x(t)$ and $y(t)$.

Child/Toy Problem

(d0 d1 d2 d3 d4)

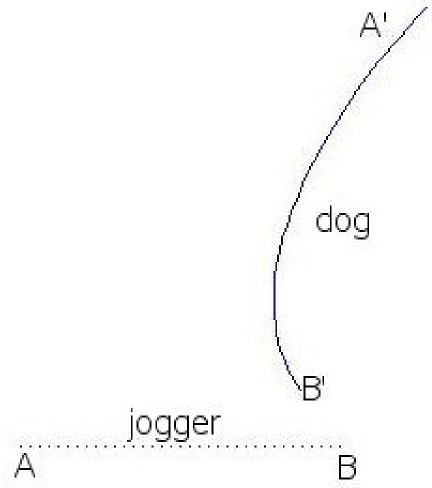


- $(X - x)^2 + (Y - y)^2 = a^2.$ bar defined by initial condition
- Toy velocity direction:

$$\mathbf{v}_T = \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \lambda \begin{pmatrix} X - x \\ Y - y \end{pmatrix} \quad \text{with} \quad \lambda > 0$$

- modulus: $||\mathbf{v}_T|| = ||\mathbf{v}_C|| \cos(\alpha) = \mathbf{v}_C \cdot \mathbf{w}$ with unit vector $\mathbf{w}$
-
```
function zs = f(t,z)
[X Xs Y Ys] = child(t); v =[Xs; Ys];
w =[X-z(1); Y-z(2)]; w = w/norm(w);
zs = (v'*w)*w;
```

Dog attacking a jogger



- Position: dog $[x(t), y(t)]$
  jogger $[X(t), Y(t)]$
- $\dot{x}^2 + \dot{y}^2 = w^2$ velocity of dog constant (maximal)
- dog's snout points always to the jogger

$$\begin{pmatrix}\dot{x}\\ \dot{y}\end{pmatrix} = \lambda \begin{pmatrix}X - x\\ Y - y\end{pmatrix} \quad \text{with } \lambda > 0$$

$$\Rightarrow w^2 = \dot{x}^2 + \dot{y}^2 = \lambda^2 \left\| \begin{pmatrix}X-x\\ Y-y\end{pmatrix} \right\|^2 \text{ and } \Rightarrow \lambda = \frac{w}{\left\| \begin{pmatrix}X-x\\ Y-y\end{pmatrix} \right\|} > 0$$

system of differential equations for dog trajectory: (d55 d5 d6 d7)

$$\begin{pmatrix}\dot{x}\\ \dot{y}\end{pmatrix} = \frac{w}{\left\| \begin{pmatrix}X - x\\ Y - y\end{pmatrix} \right\|} \begin{pmatrix}X - x\\ Y - y\end{pmatrix}$$

References

- W. Gander and D. Gruntz
  The Billiard Problem, Int. J. Math. Educ. Sci. Technol., 1992, Vol. 23, No. 6, 825-830.

- W. Gander and J. Hřebíček, ed., Solving Problems in Scientific Computing using Maple and Matlab, Springer Berlin Heidelberg New York, fourth edition 2004.

- My Home Page:

  `www.inf.ethz.ch/personal/gander/`

  or just google me!