Numerical Mathematics
Computer Arithmetic & Algebraic Equations

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Organisation

Introduction

Numerical mathematics deals with methods for the solution of problems in continuous mathematics which can be implemented on a digital computer.

Typically, use floating-point arithmetic to perform approximate calculations on real numbers.

Based on ideas and techniques from calculus and linear algebra, but yields numerical values for the solution of specific problems, rather than general formulae.
Important part of data science:

- estimate models from data,
- generate data as predictions from models, and
- compute properties of data directly.

Course

Topics

1. Computer Arithmetic & Algebraic Equations
2. Numerical Solution of Differential Equations
3. Polynomial (and Spline) Interpolation
4. Numerical Integration and Differentiation
5. Least-Squares Approximation
6. Numerical Linear Algebra

Classes Per topic: 2-3h lectures; 3-4h tutorials.
Plus: 2h revision tutorial.

Grading

80% Written exam (with calculator),

20% Homework programming assignments (4$\times$5%).

10% Homework questions (preparation for tutorial).

Regulations

Assignments The graded assignments are *individual* assignments, and follow standard DKE regulations as such.

Guidelines:

- You may not receive help solving a graded assignment from anybody else, including working together or sharing code.
- Any sources (other than the textbook, slides, the Student Portal, and other material presented in-class) must be referenced.
- You may work with other students to understand the material and on non-graded assignments (and are encouraged to do so).
- If you have written previously written code for a related problem together with other students, you should re-write the code yourself for the graded assignment.
- If you are unsure whether any work you have done together is allowed, you should declare this on your homework.

Homeworks

Homeworks *The homeworks are a vital part of the course!!! There is a* very *strong correlation between doing the homeworks and passing the course!!!!!*

Preparation You should attempt a significant proportion of the homeworks before the tutorials. Part of the grade (for DKE students) is based on preparation. This way, we can spend time going over questions which you find difficult.

Learning This course has a lot of formulae, which may seem hard at first, but don't panic! With practise, most of the questions should become routine. But you do *really* need to put the work in!

Computer use

Tutorials Bring your computer to the tutorial classes!

Matlab You are expected to have access to a computer with Matlab.

Alternatively, you may use a Matlab clone, such as GNU Octave or Scilab.

Online Learning

Instead of giving lectures in class time, I will pre-record lecture snippets.

You should read the slides and watch the snippets *before* the first class on a topic.

All class-time will be run as tutorial sessions. This will give you the maximum time to ask questions and receive feedback.

In general, during tutorials, I will answer common questions in a "plenary" session, while the teaching assistants provide individual help.

Online teaching is new to me (and new-ish to you), so this approach may change if it seems not to be working!

Mathematical Preliminaries

Calculus

- Definition of limit, derivative and integral.
- Differentiation including product and chain rules.
- Integrals of polynomials.
  - *No need to be able to perform complex integration :)*
- Intermediate value theorem and mean value theorem.
- We will cover Taylor series later!

Rate of convergence

Positive limits

Write $a_n \searrow 0$ or $a_n \to 0^+$ if all $a_n \geq 0$ and $\lim_{n\to\infty} a_n = 0$.

Big-O Notation

If $a_n, b_n \searrow 0$ as $n \to \infty$, say $a_n = O(b_n)$ if there is a constant $C > 0$ such that $a_n \leq C b_n$ for all n.

If $f, g \searrow 0$ as $h \to 0$, say $f = O(g)$ if there is a constant $C > 0$ such that $f(h) \leq C g(h)$ whenever $|h| < 1$.

Little-o Notation

Say $a_n = o(b_n)$ if $\lim_{n\to\infty} a_n/b_n = 0$.

Say $f = o(g)$ if $\lim_{h\to 0} f(h)/g(h) = 0$.

Example The sequence $a_n = \frac{2n}{n+3}$ satisfies $|a_n - 2| = \frac{6}{n+1} \leq 6 \times \frac{1}{n}$.
Hence $a_n - 2 = O(1/n)$. Say a_n converges to 2 at *rate* $O(1/n)$.

Example If $f'(x) = 0$, then $f(x+h) - f(x) = o(h)$.

Computer Arithmetic

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The answer is not exactly 0! But why does this occur??

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We shall see that the computed value of $0.6 + 0.3 + 0.1$ is *exactly* $1 - 2^{-53}$.

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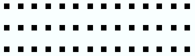
The each of these descriptions *means* "as many as ".

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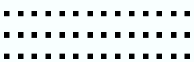
The each of these descriptions *means* "as many as ".
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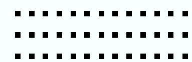
The each of these descriptions *means* "as many as ".
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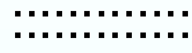
The each of these descriptions *means* "as many as ".
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Real numbers are *uncountable*, would need an *infinite* amount of data for a representation capable of describing *all* of them!

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— Requires "Computing with Infinite Data". [Now, *that's* BIG Data!!]

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— Don't round an already-rounded number!

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Example $(\frac{1}{7} + \frac{4}{7}) + \frac{2}{7} \approx (0.0010010010_2 + 0.10010010_2) + 0.010010010_2$
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The use of `format long` is vital for displaying intermediates and results of highly accurate calculations!!

Philosophical question

Philosophical question Do Klingons use floating-point?

Errors in Scientific Computing

Sources of error

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- Although we as knowledge engineers cannot do anything about these errors, we can try and estimate their impact on the final result, and maybe even choose a method which reduces this.

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$$\pi \times e^2 \stackrel{2\,\mathsf{sf}}{\approx} 3.1 \times 2.7^2 = 3.1 \times 7.29 \stackrel{2\,\mathsf{sf}}{\approx} 3.1 \times 7.3 = 22.63 \stackrel{2\,\mathsf{sf}}{\approx} 23..$$

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Relative error 19%, even though each step has a relative error of 0.1%!

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Exact value $f(x) = 1.282355$ (given by `fx`).

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Again, the accumulated error 5.3×10^{-6} is much higher than the machine epsilon for single-precision $\epsilon = 2^{-23} \approx 1.2 \times 10^{-7}$.

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Giving an answer *to higher precision than the accuracy is* useless*,*
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A certain amount of extra precision is useful in *intermediate* values to prevent unnecessary loss of accuracy when rounding.

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Reducing Errors in Scientific Computing

Subtraction

Loss of significance When subtracting two almost-equal quantities in rounded or floating-point arithmetic, many significant figures of accuracy can be lost!

Example Compute $x^3 - y^3$ using three-digit arithmetic for $x = 427$, $y = 426$.

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Exact answer 545707. High relative error of 9.9%.

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Re-write $x^3 - y^3 = (x - y) \times (x^2 + xy + y^2)$.

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Example Compute $x^3 - y^3$ using three-digit arithmetic for $x = 427$, $y = 426$.

$$x^3 - y^3 = 427^3 - 426^3 = 77854483 - 77308776$$
$$\overset{3\,\mathrm{sf}}{\approx} 77900000 - 77300000 = 600000 \overset{3\,\mathrm{sf}}{=} 6.00 \times 10^5.$$

Exact answer 545707. High relative error of 9.9%.

Re-write $x^3 - y^3 = (x - y) \times (x^2 + xy + y^2)$. Then

$$x^3 - y^3 = (427 - 426) \times (427^2 + 427 \times 426 + 426^2)$$

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Exact answer 545707. Relative error $1.3\times 10^{-3} = 0.13\%$.

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Safe subtraction Subtraction of *exact* values *at the first step* is safe! This is because errors have not had a chance to accumulate.

Subtraction

Example Now compute $x^3 - y^3$ using single-precision arithmetic for the values $x = 427$, $y = 426$.

$$\begin{aligned} x^3 - y^3 = 427^3 - 426^3 &= 77854483 - 77308776 \\ &\overset{\text{sp}}{\approx} 77854480 - 77308776 = 545704 \overset{\text{sp}}{=} 545704. \end{aligned}$$

Exact answer 545707. Relative error 5.5×10^{-6}.

Re-write $x^3 - y^3 = (x - y) \times (x^2 + xy + y^2)$. Then

$$\begin{aligned} x^3 - y^3 &= (427 - 426) \times (427^2 + 427! \times 426 + 426^2) \\ &= 1 \times (182329 + 181902 + 181476) \\ &\overset{\text{sp}}{\approx} 1 \times (182329 + 181902 + 181476) = 545707 \overset{\text{sp}}{\approx} 545707. \end{aligned}$$

Answer is exact!

Quadratic formula

Problem Compute the positive root of $0.5x^2 + 2x - 0.05$ using 3-digit arithmetic.

Quadratic formula

Problem Compute the positive root of $0.5x^2 + 2x - 0.05$ using 3-digit arithmetic.

Use the quadratic formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

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$$\begin{aligned} b^2 - 4ac &= 2^2 - 4 \times 0.5 \times (-0.05) = 4 \times (-0.1) = 4.1, \\ 2a &= 2 \times 0.5 = 1, \end{aligned}$$

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Exact answer $0.02484567\cdots = 0.0248$ $(3\,\text{sf})$.

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Exact answer $0.02484567 \cdots = 0.0248\ (3\,\text{sf})$.

Absolute error $|0.02 - 0.02484567| = 0.00484567 \cdots = 0.0048\ (2\,\text{sf})$.

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Exact answer $0.02484567\cdots = 0.0248\;(3\,\text{sf})$.

Absolute error $|0.02 - 0.02484567| = 0.00484567\cdots = 0.0048\,(2\,\text{sf})$.
Relative error $|0.00484567|/|0.02484567| = 0.195031\cdots = 0.20\,(2\,\text{sf}) \approx 20\%$!!

Quadratic formula

Rearrange the formula by completing the square:

$$
\begin{aligned}
x = \frac{\sqrt{b^2 - 4ac} - b}{2a} &= \frac{\sqrt{b^2 - 4ac} - b}{2a} \times \frac{\sqrt{b^2 - 4ac} + b}{\sqrt{b^2 - 4ac} + b} \\
&= \frac{(b^2 - 4ac) - b^2}{2a(\sqrt{b^2 - 4ac} + b)} = \frac{-4ac}{2a(\sqrt{b^2 - 4ac} + b)} \\
&= \frac{-2c}{\sqrt{b^2 - 4ac} + b}
\end{aligned}
$$

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Rearrange the formula by completing the square:

$$\begin{aligned} x &= \frac{\sqrt{b^2-4ac}-b}{2a} = \frac{\sqrt{b^2-4ac}-b}{2a} \times \frac{\sqrt{b^2-4ac}+b}{\sqrt{b^2-4ac}+b} \\ &= \frac{(b^2-4ac)-b^2}{2a(\sqrt{b^2-4ac}+b)} = \frac{-4ac}{2a(\sqrt{b^2-4ac}+b)} \\ &= \frac{-2c}{\sqrt{b^2-4ac}+b} \end{aligned}$$

Example Compute the positive root of $0.5x^2+2x-0.05$ using 3-digit arithmetic.

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$$
x = \frac{-2c}{\sqrt{b^2-4ac}+b} = \frac{-2\times(-0.05)}{\sqrt{4.1}+2} = \frac{0.1}{2.02\cancel{498\cdots}+2}
$$

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Rearrange the formula by completing the square:

$$\begin{aligned} x &= \frac{\sqrt{b^2-4ac}-b}{2a} = \frac{\sqrt{b^2-4ac}-b}{2a} \times \frac{\sqrt{b^2-4ac}+b}{\sqrt{b^2-4ac}+b} \\ &= \frac{(b^2-4ac)-b^2}{2a(\sqrt{b^2-4ac}+b)} = \frac{-4ac}{2a(\sqrt{b^2-4ac}+b)} \\ &= \frac{-2c}{\sqrt{b^2-4ac}+b} \end{aligned}$$

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&\overset{3\,\text{sf}}{\approx} \frac{0.1}{2.02+2} = 0.1/4.02 = 0.0248756\cdots \overset{3\,\text{sf}}{\approx} 0.0249.
\end{aligned}
$$

Quadratic formula

Rearrange the formula by completing the square:

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Exact answer $x = 0.02484567\cdots = 0.0248\,(3\,\text{sf})$.

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Rearrange the formula by completing the square:

$$\begin{aligned} x &= \frac{\sqrt{b^2-4ac}-b}{2a} = \frac{\sqrt{b^2-4ac}-b}{2a} \times \frac{\sqrt{b^2-4ac}+b}{\sqrt{b^2-4ac}+b} \\ &= \frac{(b^2-4ac)-b^2}{2a(\sqrt{b^2-4ac}+b)} = \frac{-4ac}{2a(\sqrt{b^2-4ac}+b)} \\ &= \frac{-2c}{\sqrt{b^2-4ac}+b} \end{aligned}$$

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$$x = \frac{-2c}{\sqrt{b^2-4ac}+b} = \frac{-2\times(-0.05)}{\sqrt{4.1}+2} = \frac{0.1}{2.02\cancel{498\cdots}+2}$$

$$\stackrel{3\,\text{sf}}{\approx} \frac{0.1}{2.02+2} = 0.1/4.02 = 0.0248756\cdots \stackrel{3\,\text{sf}}{\approx} 0.0249.$$

Exact answer $x = 0.02484567\cdots = 0.0248\,(3\,\text{sf})$.

Absolute error $|0.0249 - 0.02484567| = 0.00054326\cdots = 0.00054\,(2\,\text{sf})$.

Quadratic formula

Rearrange the formula by completing the square:

$$
\begin{aligned}
x = \frac{\sqrt{b^2-4ac}-b}{2a} &= \frac{\sqrt{b^2-4ac}-b}{2a} \times \frac{\sqrt{b^2-4ac}+b}{\sqrt{b^2-4ac}+b} \\
&= \frac{(b^2-4ac)-b^2}{2a(\sqrt{b^2-4ac}+b)} = \frac{-4ac}{2a(\sqrt{b^2-4ac}+b)} \\
&= \frac{-2c}{\sqrt{b^2-4ac}+b}
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Example Compute the positive root of $0.5x^2 + 2x - 0.05$ using 3-digit arithmetic.

$$
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&\overset{3\,\text{sf}}{\approx} \frac{0.1}{2.02+2} = 0.1/4.02 = 0.0248756\cdots \overset{3\,\text{sf}}{\approx} 0.0249.
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$$

Exact answer $x = 0.02484567\cdots = 0.0248\,(3\,\text{sf})$.

Absolute error $|0.0249 - 0.02484567| = 0.00054326\cdots = 0.00054\,(2\,\text{sf})$.

Relative error $|0.00054326|/|0.02484567| = 0.002187\cdots = 0.0021\,(2\,\text{sf}) \approx 0.2\%$

Polynomials in Horner nested form

Problem Evaluate $f(x) = x^3 - 5.34x^2 + 1.52x + 4.61$ at $x = 4.89$ using 3-digit arithmetic.

Polynomials in Horner nested form

Problem Evaluate $f(x) = x^3 - 5.34x^2 + 1.52x + 4.61$ at $x = 4.89$ using 3-digit arithmetic.

We previously found $f(x) \approx 1.04$ by direct evaluation; relative error 19%.

Polynomials in Horner nested form

Problem Evaluate $f(x) = x^3 - 5.34x^2 + 1.52x + 4.61$ at $x = 4.89$ using 3-digit arithmetic.

Re-write in *nested form* (also known as *Horner's rule*):

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Re-write in *nested form* (also known as *Horner's rule*):

$$x^3 - 5.34x^2 + 1.52x + 4.61 = (x^2 - 5.34x + 1.52) \cdot x + 4.61$$

Polynomials in Horner nested form

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Re-write in *nested form* (also known as *Horner's rule*):

$$
\begin{aligned}
x^3 - 5.34x^2 + 1.52x + 4.61 &= (x^2 - 5.34x + 1.52) \cdot x + 4.61 \\
&= \big((x - 5.34) \cdot x + 1.52\big) \cdot x + 4.61
\end{aligned}
$$

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Re-write in *nested form* (also known as *Horner's rule*):

$$\begin{aligned} x^3 - 5.34x^2 + 1.52x + 4.61 &= (x^2 - 5.34x + 1.52) \cdot x + 4.61 \\ &= \big((x - 5.34) \cdot x + 1.52\big) \cdot x + 4.61 \end{aligned}$$

$f(4.89) = ((4.89 - 5.34) \times 4.89 + 1.52) \times 4.89 + 4.61$

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Problem Evaluate $f(x) = x^3 - 5.34x^2 + 1.52x + 4.61$ at $x = 4.89$ using 3-digit arithmetic.

Re-write in *nested form* (also known as *Horner's rule*):

$$\begin{aligned} x^3 - 5.34x^2 + 1.52x + 4.61 &= (x^2 - 5.34x + 1.52) \cdot x + 4.61 \\ &= \big((x - 5.34) \cdot x + 1.52\big) \cdot x + 4.61 \end{aligned}$$

$$\begin{aligned} f(4.89) &= ((4.89 - 5.34) \times 4.89 + 1.52) \times 4.89 + 4.61 \\ &= (-0.45 \times 4.89 + 1.52) \times 4.89 + 4.61 \end{aligned}$$

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$$\begin{aligned} x^3 - 5.34x^2 + 1.52x + 4.61 &= (x^2 - 5.34x + 1.52) \cdot x + 4.61 \\ &= \big((x - 5.34) \cdot x + 1.52\big) \cdot x + 4.61 \end{aligned}$$

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c=[1.0,-5.34,1.52,4.61]
fdirect = @(x) c(1)*x^3 + c(2)*x^2 + c(3)*x + c(4)
fnested = @(x) ((c(1)*x+c(2))*x+c(3))*x+c(4)
fdirectrounded = @(x) r(r(r(r(r(x*x)*x)-r(5.34*r(x*x)))
                        +r(1.52*x))+4.61)
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```
xr=Rounded(x,3)
ydr=fdirect(xr); ydr.value
ynr=fnested(xr); ynr.value
```

Nested form

The nested form of

$$\sum_{k=0}^{n} a_k x^k = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_2 x^2 + a_1 x + a_0$$

is

$$\Big(\Big((\cdots(a_n\, x + a_{n-1}) \cdot x + \cdots) \cdot x + a_2) \cdot x + a_1) \cdot x + a_0\Big)\Big)$$

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Here, the formula is simply evaluated from left to right.

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$$\sum_{k=0}^{n} = a_0 + x \cdot \Big(a_1 + x \cdot \Big(a_2 + x \cdot (\cdots + x \cdot (a_{n-1} + x \cdot a_n) \cdots)\Big)\Big)$$

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e.g. For $n = 5$,

$$\begin{aligned} & a_5 x^5 + a_4 x^4 + a_3 x^3 + a_2 x^2 + a_1 x + a_0 \\ & \qquad = ((((a_5 \cdot x + a_4) \cdot x + a_3) \cdot x + a_2) \cdot x + a_1) \cdot x + a_0 \\ & \qquad = a_0 + x \cdot (a_1 + x \cdot (a_2 + x \cdot (a_3 + x \cdot (a_4 + x \cdot a_5)))) \end{aligned}$$

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e.g. Horner's method does not *always* give a more accurate result than direct evaluation, does not have as bad a worst-case.

Solutions of Equations of One Variable

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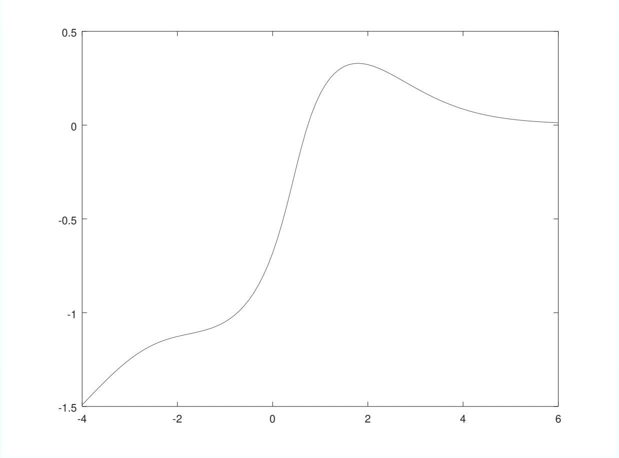
Approach Fix x-values $(x_0, x_1, \ldots, x_n)$, and try to find y-values $(y_0, y_1, \ldots, y_n)$. i.e. Solve equation of the form $f(x_i, y) = 0$ to find y_i.



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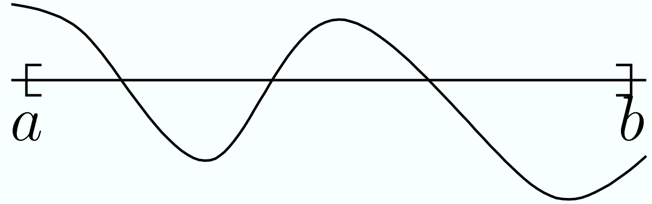

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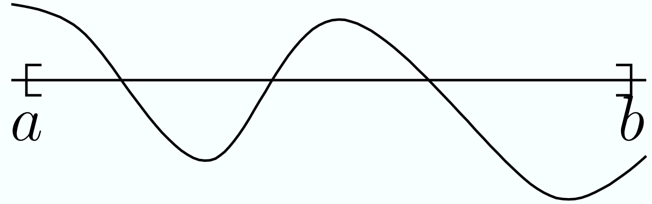

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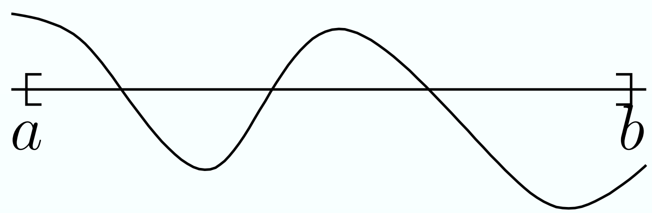

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Signs Note that if $f(a), f(b) \neq 0$, then

$$\operatorname{sgn}(f(a)) \neq \operatorname{sgn}(f(b)) \iff f(a)f(b) < 0.$$

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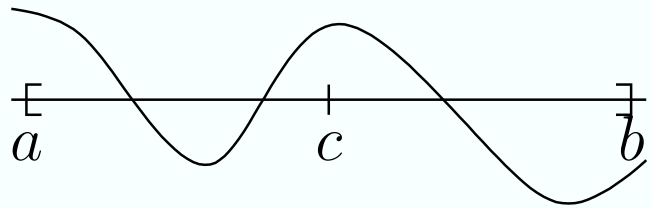

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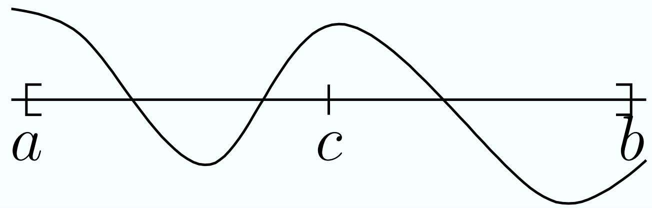

Update $a := c$ if $\operatorname{sgn}(f(a)) = \operatorname{sgn}(f(c)) \neq \operatorname{sgn}(f(b))$,
or $b := c$ if $\operatorname{sgn}(f(a)) \neq \operatorname{sgn}(f(c)) = \operatorname{sgn}(f(b))$.

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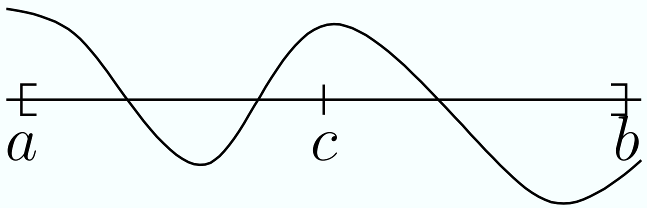

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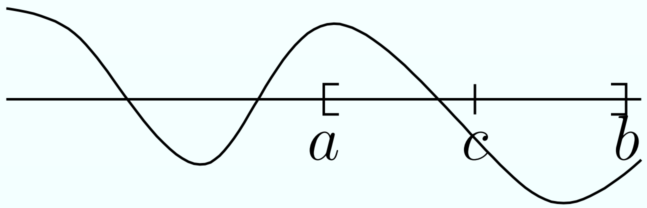

The bisection method

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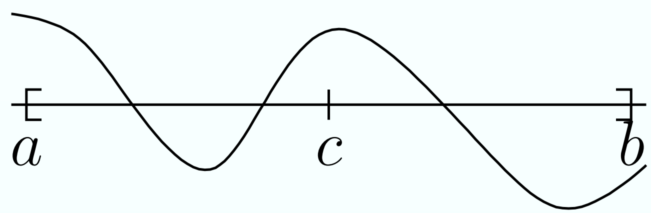

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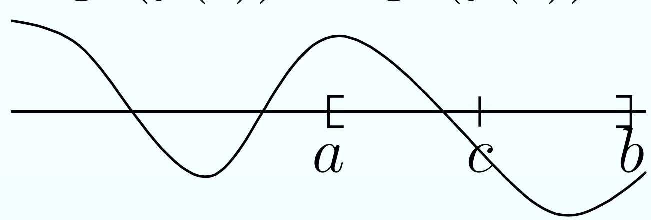

The width of the interval $[a, b]$ is halved.

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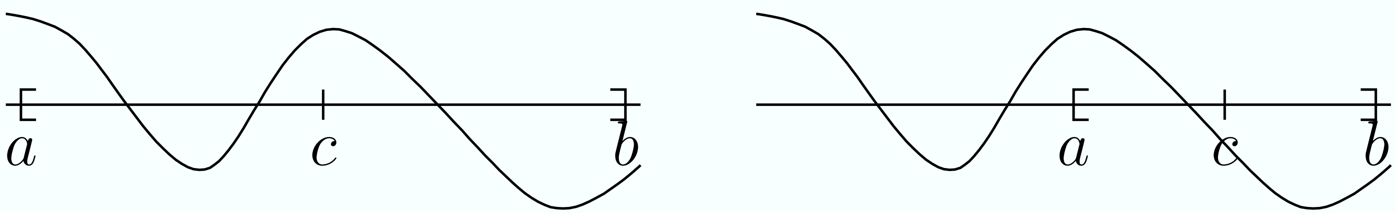

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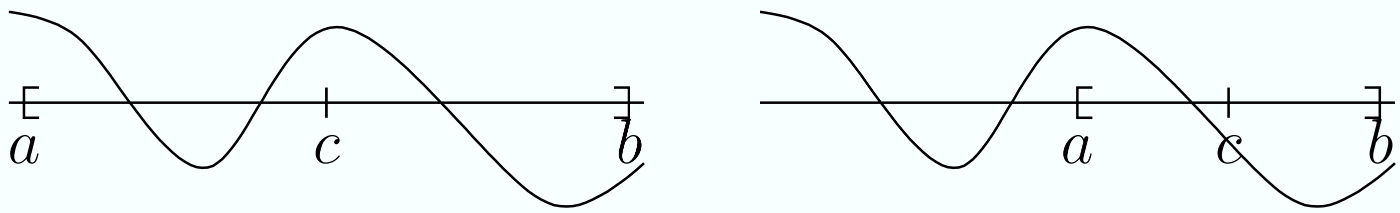

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If the radius of $[a, b]$, which is given by $\dfrac{b-a}{2}$, is less than ϵ, then any point in $[a, b]$, *including the root p,* is within ϵ of the midpoint c.

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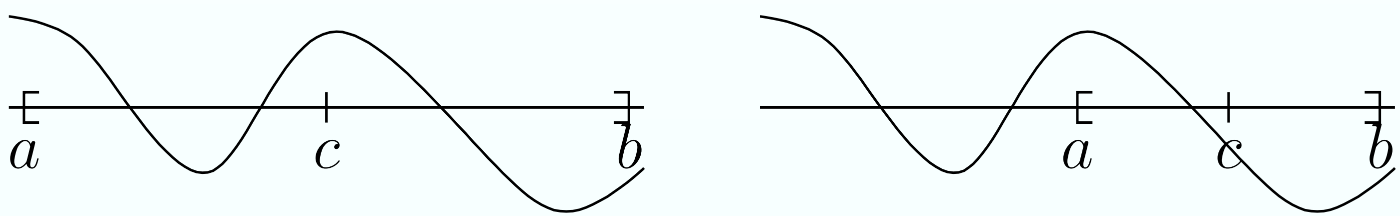

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Taking $p^* = (a+b)/2$ then yields $|p^* - p| < \epsilon$.

Iterative methods

Iterative methods The bisection method is an *iterative* method: we apply the same steps over and over again.

Iterative methods are typically implemented as a loop:

input f, a, b, ϵ such that $\mathrm{sgn}(f(a)) \neq \mathrm{sgn}(f(b)) < 0$ and $\epsilon > 0$. while $(b-a)/2 > \epsilon$,

$c := (a+b)/2$;

if $\mathrm{sgn}(f(c)) = \mathrm{sgn}(f(a))$

then $a := c,\ b := b$

else $a := a,\ b := c$

end if

end while

$r := (a+b)/2$

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Here, we *overwrite* variables as they are no longer needed.

Iterative methods

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Indexed values In mathematical work, or if a record of previous values is needed, we often *index* the variables by the loop-count:

input f, a_0, b_0, ϵ such that $\operatorname{sgn}(f(a_0)) \neq \operatorname{sgn}(f(b))$ and $\epsilon > 0$. n:=0;

while $(b_n - a_n)/2 > \epsilon$,

$c_n := (a_n + b_n)/2;$

if $\operatorname{sgn}(f(c_n)) = \operatorname{sgn}(f(a_n))$

then $a_{n+1} := c_n,\ b_{n+1} := b_n$

else $a_{n+1} := a_n,\ b_{n+1} := c_n$

end if

$n := n + 1$

end while

$r := (a_n + b_n)/2$

The bisection method

Example Estimate $\sqrt{2}$ to within 0.1.

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Compute $f(c) = f(1.5) = 1.5^2 - 2 = 2.25 - 2 = 0.25$.

Since $f(c) > 0$ has the opposite sign to $f(a)$, keep $a = 1.0$ and set $b := c = 1.5$.

The bisection method

Example Estimate $\sqrt{2}$ to within 0.1.

Continue by finding a root of $f(x) = x^2 - 2$ in the interval $[a, b] = [1.0, 1.5]$.

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Set $c = \frac{a+b}{2} = \frac{1.0+1.5}{2} = 1.25$.

Compute $f(c) = 1.25^2 - 2 = 1.5625 - 2 = -0.4375$.

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Continue by finding a root of $f(x) = x^2 - 2$ in the interval $[a, b] = [1.0, 1.5]$.

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Compute $f(c) = 1.25^2 - 2 = 1.5625 - 2 = -0.4375$.

Since $f(c) < 0$ has the opposite sign to $f(b)$,
set $a := c = 1.25$ and keep $b = 1.5$.

Set $c = \frac{a+b}{2} = \frac{1.25+1.5}{2} = 1.375$.

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Since $f(c) < 0$ has the opposite sign to $f(b)$,
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Since $(b - a)/2 = (1.5 - 1.375)/2 = 0.0625 < 0.1$, taking $p^* = 1.4375$, the midpoint of $[a, b]$, means $|p^* - \sqrt{2}| < 0.0625 < 0.1$.

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In fact, $|p^* - \sqrt{2}| = 0.023$ (2sf)

The bisection method-Example (Complete)

Example Estimate $\sqrt{2}$ to within 0.1.

Start with $a_0 = 1$ and $b_0 = 2$.

Set $c_0 = 1.5$ with $f(c_0) = 0.25 > 0$,
so f has a root in $[a_0, c_0] = [1, 1.5]$.

Update $a_1 = a_0 = 1.0$, $b_1 = c_0 = 1.5$.

Set $c_1 = \frac{a_1+b_1}{2} = \frac{1.0+1.5}{2} = 1.25$

Compute $f(c_1) = -0.4375 < 0$,
so f has a root in $[c_1, b_1] = [1.25, 1.5]$.

Update $a_2 = c_1 = 1.25$, $b_2 = b_1 = 1.5$.

Set $c_2 = \frac{a_2+b_2}{2} = \frac{1.25+1.5}{2} = 1.375$.

Since $f(c_2) = f(1.375) = -0.109375 < 0$,
f has a root in $[c_2, b_2] = [1.375, 1.5]$.

Update $a_3 = c_2 = 1.375$, $b_3 = b_2 = 1.5$.

$f(1) = 1^2 - 2 = -1$

$f(2) = 2^2 - 2 = 2$

$f(1.5) = 1.5^2 - 2$
$= 2.25 - 2 = 0.25$

$f(1.25) = 1.25^2 - 2$
$= 1.5625 - 2$
$= -0.4375$

$f(1.375) = 1.375^2 - 2$
$= 1.890625 - 2$
$= -0.109375$

Since $(b_3 - a_3)/2 = (1.5 - 1.375)/2 = 0.0625 < 0.1$, taking $p^* = 1.4375$, the midpoint of $[a_3, b_3] = [1.375, 1.5]$, means $|p^* - \sqrt{2}| < 0.0625 < 0.1$.

The bisection method

Implementation In file `bisection_root.m`

```
function r=bisection_root(f,a,b,e)
% Solve f(x)=0 for x in [a,b] up to a tolerance of e.
    assert a<b; assert e>0;
    assert sign(f(a))==-sign(f(b));
    while (b-a)/2 > e,
        c=(a+b)/2;
        if sign(f(c))==sign(f(a)),
            then a=c;
            else b=c;
        endif
    endwhile
    r=(a+b)/2;
endfunction
```

Usage In a separate script file e.g. `sqrt_two.m`

```
f=@(x)x^2-2; a=1; b=2; tol=0.1;
r=bisection_root(f, a, b, tol)
```

The bisection method

Convergence Since the error halves at each step, the method obtains an approximation to within tolerance ϵ in n steps, where $\frac{1}{2}(b-a)/2^n < \epsilon$, or

$$n > \log_2\bigl((b-a)/2\epsilon\bigr) = O(\log_2(1/\epsilon)).$$

Note $\log_2(x) = \ln(x)/\ln(2)$ where $\ln$ is the natural logarithm.

Example To find a root of f in $[1, 2]$ to tolerance $\epsilon = 0.1$, need

$$n > \log_2\bigl((2-1)/(2\times 0.1)\bigr) = \log_2(5) \approx 2.3,$$

so take $n = 3$ steps.

The secant method

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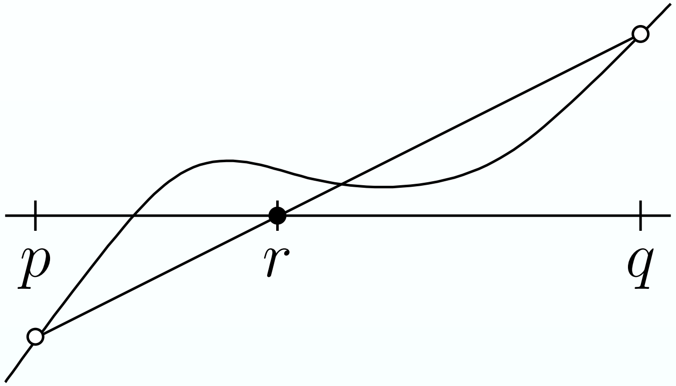
Idea Given approximations p, q to a root of f, approximate f by the line joining $(p, f(p))$ and $(q, f(q))$.



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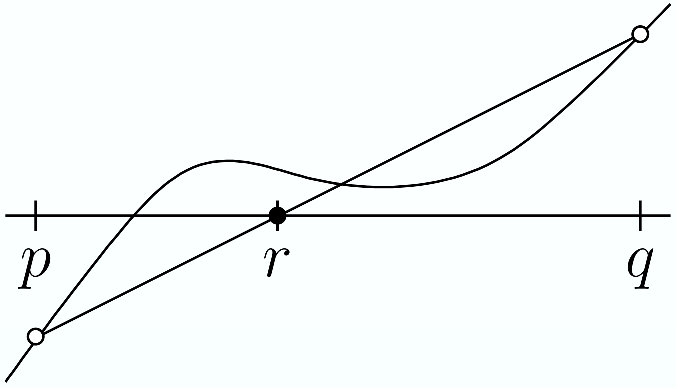

Obtain a better approximation $r = S(f, p, q)$ to the root by finding where this line crosses the x-axis.

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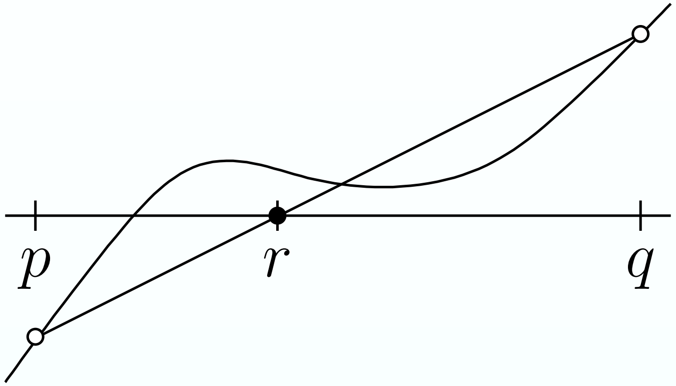

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Starting from initial points p_0, p_1, iteratively compute $p_2 = S(f, p_0, p_1)$, $p_3 = S(f, p_1, p_2), \ldots$.

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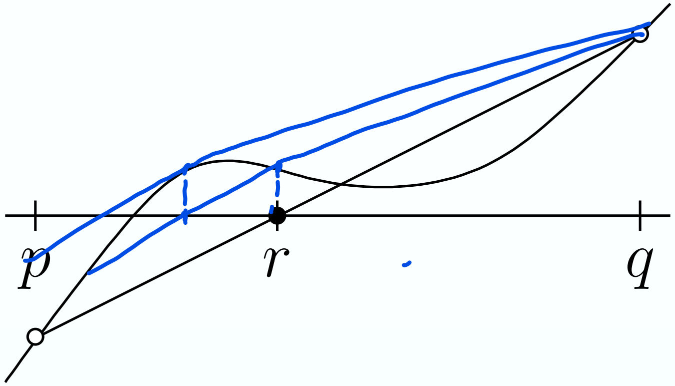

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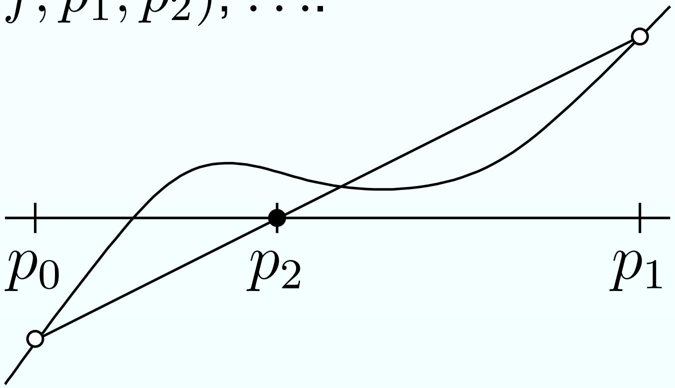

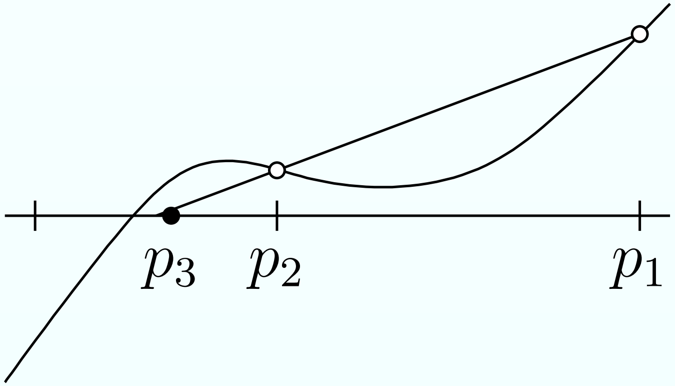

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Algorithm Apply as an iterative algorithm. Start with p_0, p_1, and set

$$\boxed{p_{n+1} = p_n - \frac{p_n - p_{n-1}}{f(p_n) - f(p_{n-1})} f(p_n).}$$

Bracketing The points p_n, p_{n+1} do *not* need to bracket a root!

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

The secant method

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Secant method iterative formula:

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We will work to machine precision, displaying intermediates to 3 decimal places.

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Initial step computes p_2 by taking $n = 1$ in general formula.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1)$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

Secant method iterative formula:

$$p_{n+1} = p_n - \frac{p_n - p_{n-1}}{f(p_n) - f(p_{n-1})} f(p_n)$$

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Initial step computes p_2 by taking $n = 1$ in general formula.
Need $f(p_0) = f(1) = -1.000$ and $f(p_1) = f(2) = 2.000$.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1)$$

The secant method

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$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1) = 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000$$

The secant method

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$$= 2.000 - \frac{1.000}{3.000} \times 2.000$$

The secant method

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$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

Secant method iterative formula:

$$p_{n+1} = p_n - \frac{p_n - p_{n-1}}{f(p_n) - f(p_{n-1})} f(p_n)$$

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$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1) = 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000$$

$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667 = 1.333 \ (3\,\text{dp})$$

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$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667 = 1.333 \ (3\,\text{dp})$$

Second step computes p_3 by taking $n = 2$ in formula.

The secant method

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Secant method iterative formula:

$$p_{n+1} = p_n - \frac{p_n - p_{n-1}}{f(p_n) - f(p_{n-1})} f(p_n)$$

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Second step computes p_3 by taking $n = 2$ in formula.

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2)$$

The secant method

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$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667 = 1.333 \ (3\,\text{dp})$$

Second step computes p_3 by taking $n = 2$ in formula. Need $f(p_2) = -0.222$.

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2)$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

Secant method iterative formula:

$$p_{n+1} = p_n - \frac{p_n - p_{n-1}}{f(p_n) - f(p_{n-1})} f(p_n)$$

We will work to machine precision, displaying intermediates to 3 decimal places.

Initial step computes p_2 by taking $n = 1$ in general formula.
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$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667 = 1.333 \ (3\,\text{dp})$$

Second step computes p_3 by taking $n = 2$ in formula. Need $f(p_2) = -0.222$.

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2) \overset{3\,\text{dp}}{=} 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222)$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

Secant method iterative formula:

$$p_{n+1} = p_n - \frac{p_n - p_{n-1}}{f(p_n) - f(p_{n-1})} f(p_n)$$

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$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667 = 1.333 \text{ (3 dp)}$$

Second step computes p_3 by taking $n = 2$ in formula. Need $f(p_2) = -0.222$.

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2) \overset{3\,\text{dp}}{=} 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222)$$

$$= 1.333 - \frac{-0.667}{-2.222}(-0.222)$$

The secant method

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$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1) = 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000$$

$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667 = 1.333 \ (3\,\text{dp})$$

Second step computes p_3 by taking $n = 2$ in formula. Need $f(p_2) = -0.222$.

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2) \overset{3\,\text{dp}}{=} 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222)$$

$$= 1.333 - \frac{-0.667}{-2.222}(-0.222) = 1.333 - (-0.0667)$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

Secant method iterative formula:

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We will work to machine precision, displaying intermediates to 3 decimal places.

Initial step computes p_2 by taking $n = 1$ in general formula.
Need $f(p_0) = f(1) = -1.000$ and $f(p_1) = f(2) = 2.000$.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1) = 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000$$

$$= 2.000 - \frac{1.000}{3.000} \times 2.000 = 2.000 - 0.667 = 1.333 \ (3\,\text{dp})$$

Second step computes p_3 by taking $n = 2$ in formula. Need $f(p_2) = -0.222$.

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2) \overset{3\,\text{dp}}{=} 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222)$$

$$= 1.333 - \frac{-0.667}{-2.222}(-0.222) = 1.333 - (-0.0667) = 1.400.$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$f(p_0) = f(1.000) = -1.000$$

$$f(p_1) = f(2.000) = 2.000$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1)$$

$$= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333$$

$$f(p_0) = f(1.000) = -1.000$$

$$f(p_1) = f(2.000) = 2.000$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$
\begin{aligned}
p_2 &= p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1) \\
&= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333
\end{aligned}
$$

$$f(p_0) = f(1.000) = -1.000$$

$$f(p_1) = f(2.000) = 2.000$$

$$
\begin{aligned}
f(p_2) &= f(1.333) = 1.333^2 - 2 \\
&= 1.778 - 2 = -0.222
\end{aligned}
$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1)$$

$$= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333$$

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2)$$

$$= 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222) = 1.400$$

$$f(p_0) = f(1.000) = -1.000$$

$$f(p_1) = f(2.000) = 2.000$$

$$f(p_2) = f(1.333) = 1.333^2 - 2$$

$$= 1.778 - 2 = -0.222$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1)$$
$$= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333$$

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2)$$
$$= 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222) = 1.400$$

$$f(p_0) = f(1.000) = -1.000$$
$$f(p_1) = f(2.000) = 2.000$$
$$f(p_2) = f(1.333) = 1.333^2 - 2$$
$$= 1.778 - 2 = -0.222$$
$$f(p_3) = f(1.400) = 1.400^2 - 2$$
$$= 1.9600 - 2 = -0.0400$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$
\begin{aligned}
p_2 &= p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1) \\
&= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333 \\
p_3 &= p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2) \\
&= 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222) = 1.400 \\
p_4 &= 1.4000 - \frac{1.4000 - 1.3333}{-0.0400 - (-0.2222)} \times (-0.0400) \\
&= 1.4000 - (-0.0146) = 1.4146 \ (4\,\text{dp})
\end{aligned}
$$

$$
\begin{aligned}
f(p_0) &= f(1.000) = -1.000 \\
f(p_1) &= f(2.000) = 2.000 \\
f(p_2) &= f(1.333) = 1.333^2 - 2 \\
&= 1.778 - 2 = -0.222 \\
f(p_3) &= f(1.400) = 1.400^2 - 2 \\
&= 1.9600 - 2 = -0.0400
\end{aligned}
$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1)$$
$$= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333$$

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2)$$
$$= 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222) = 1.400$$

$$p_4 = 1.4000 - \frac{1.4000 - 1.3333}{-0.0400 - (-0.2222)} \times (-0.0400)$$
$$= 1.4000 - (-0.0146) = 1.4146 \ (4\,\text{dp})$$

$$f(p_0) = f(1.000) = -1.000$$
$$f(p_1) = f(2.000) = 2.000$$
$$f(p_2) = f(1.333) = 1.333^2 - 2$$
$$= 1.778 - 2 = -0.222$$
$$f(p_3) = f(1.400) = 1.400^2 - 2$$
$$= 1.9600 - 2 = -0.0400$$
$$f(p_4) = f(1.4146) = -0.00119$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$p_2 = p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1)$$

$$= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333$$

$$p_3 = p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2)$$

$$= 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222) = 1.400$$

$$p_4 = 1.4000 - \frac{1.4000 - 1.3333}{-0.0400 - (-0.2222)} \times (-0.0400)$$

$$= 1.4000 - (-0.0146) = 1.4146 \ (4\,\text{dp})$$

$$p_5 = 1.41463 - \frac{1.41463 - 1.40000}{0.00119 - (-0.0400)} \times (0.00119)$$

$$= 1.41463 - 0.00042 = 1.41421 \ (5\,\text{dp})$$

$$f(p_0) = f(1.000) = -1.000$$

$$f(p_1) = f(2.000) = 2.000$$

$$f(p_2) = f(1.333) = 1.333^2 - 2$$
$$= 1.778 - 2 = -0.222$$

$$f(p_3) = f(1.400) = 1.400^2 - 2$$
$$= 1.9600 - 2 = -0.0400$$

$$f(p_4) = f(1.4146) = -0.00119$$

The secant method

Example Solve $f(x) = x^2 - 2 = 0$. Start with $p_0 = 1$, $p_1 = 2$.

$$
\begin{aligned}
p_2 &= p_1 - \frac{p_1 - p_0}{f(p_1) - f(p_0)} f(p_1) \\
&= 2.000 - \frac{2.000 - 1.000}{2.000 - (-1.000)} \times 2.000 = 1.333 \\
p_3 &= p_2 - \frac{p_2 - p_1}{f(p_2) - f(p_1)} f(p_2) \\
&= 1.333 - \frac{1.333 - 2.000}{-0.222 - 2.000} \times (-0.222) = 1.400 \\
p_4 &= 1.4000 - \frac{1.4000 - 1.3333}{-0.0400 - (-0.2222)} \times (-0.0400) \\
&= 1.4000 - (-0.0146) = 1.4146 \ (4\,\text{dp}) \\
p_5 &= 1.41463 - \frac{1.41463 - 1.40000}{0.00119 - (-0.0400)} \times (0.00119) \\
&= 1.41463 - 0.00042 = 1.41421 \ (5\,\text{dp})
\end{aligned}
$$

$$
\begin{aligned}
f(p_0) &= f(1.000) = -1.000 \\
f(p_1) &= f(2.000) = 2.000 \\
f(p_2) &= f(1.333) = 1.333^2 - 2 \\
&= 1.778 - 2 = -0.222 \\
f(p_3) &= f(1.400) = 1.400^2 - 2 \\
&= 1.9600 - 2 = -0.0400 \\
f(p_4) &= f(1.4146) = -0.00119 \\
f(p_5) &= f(1.414211) \\
&= -0.0000060
\end{aligned}
$$

Stopping criteria

Convergence Want to stop when $|p_n - p| < \epsilon$.

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Problem

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Problem Don't know exact root p!

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If convergence is rapid, expect $|p_n - p| \ll |p_{n-1} - p|$.

Stopping criteria

Convergence Want to stop when $|p_n - p| < \epsilon$.

Problem Don't know exact root p!

If convergence is rapid, expect $|p_n - p| \ll |p_{n-1} - p|$.

If $|p_n - p| = \frac{1}{\gamma}|p_{n-1} - p|$ with $\frac{1}{\gamma} \leq \frac{1}{2}$, find $|p_{n-1} - p_n| \geq |p - p_n|$.

Stopping criteria

Convergence Want to stop when $|p_n - p| < \epsilon$.

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If convergence is rapid, expect $|p_n - p| \ll |p_{n-1} - p|$.

If $|p_n - p| = \frac{1}{\gamma}|p_{n-1} - p|$ with $\frac{1}{\gamma} \leq \frac{1}{2}$, find $|p_{n-1} - p_n| \geq |p - p_n|$.

Practical stopping heuristic $\boxed{\text{Stop when } |p_n - p_{n-1}| < \epsilon.}$

Stopping criteria

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If convergence is rapid, expect $|p_n - p| \ll |p_{n-1} - p|$.

If $|p_n - p| = \frac{1}{\gamma}|p_{n-1} - p|$ with $\frac{1}{\gamma} \leq \frac{1}{2}$, find $|p_{n-1} - p_n| \geq |p - p_n|$.

Practical stopping heuristic $\boxed{\text{Stop when } |p_n - p_{n-1}| < \epsilon.}$

Error estimate For the heuristic $|p_n - p_{n-1}| < \epsilon$, expect $|p_n - p| \lesssim \epsilon$.

Stopping criteria

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Problem Don't know exact root p!

If convergence is rapid, expect $|p_n - p| \ll |p_{n-1} - p|$.

If $|p_n - p| = \frac{1}{\gamma}|p_{n-1} - p|$ with $\frac{1}{\gamma} \leq \frac{1}{2}$, find $|p_{n-1} - p_n| \geq |p - p_n|$.

Practical stopping heuristic $\boxed{\text{Stop when } |p_n - p_{n-1}| < \epsilon.}$

Error estimate For the heuristic $|p_n - p_{n-1}| < \epsilon$, expect $|p_n - p| \lesssim \epsilon$.

Error bound If also $f(p_n)$ and $f(p_{n-1})$ have different signs, then $|p_n - p| < \epsilon$.

Stopping criteria

Example Solve $x^2 - 2 = 0$ to an accuracy of 0.01.

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Check differences:

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So we can *expect* $|p_5 - \sqrt{2}| < 0.01$.

Solution $\sqrt{2} \approx p_5 = 1.4142$ $(4\,\text{dp}) = 1.41$ $(2\,\text{dp})$.

Note: Actual error $|p_5 - \sqrt{2}| = |1.4142 - \sqrt{2}| \approx 2.1 \times 10^{-4} \ll 0.01$.

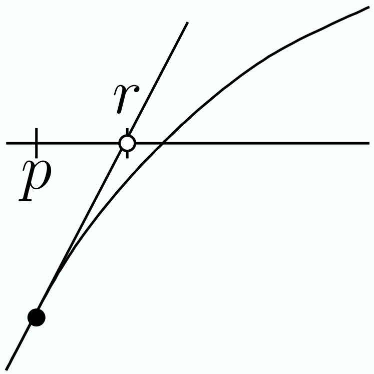
The secant method

Implementation

```
function r=secant(f,p,q,e)
    while abs(q-p) > e,
        r = ... ;
        p = q; q=r;
    endwhile
endfunction
```

Newton-Raphson method

Idea Instead of using the secant line joining $(p, f(p))$ and $(q, f(q))$, use the tangent line at $(p, f(p))$



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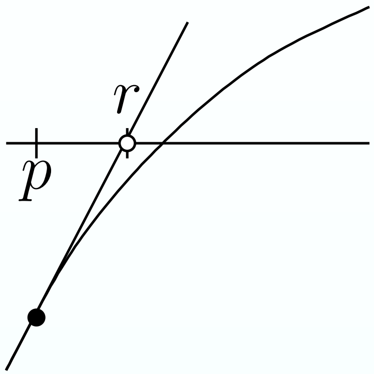

Tangent line at $(p, f(p))$ has equation $y = f(p) + f'(p)\,(x - p)$.

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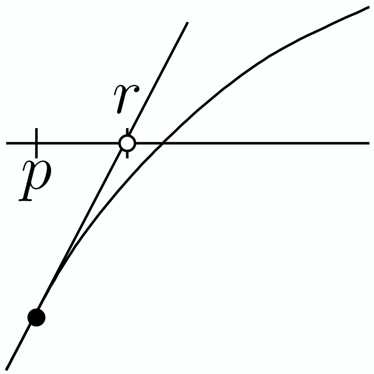

Tangent line at $(p, f(p))$ has equation $y = f(p) + f'(p)\,(x - p)$.

Setting $y = 0$ and solving for $r = x$ gives intercept at $r = p - f(p)/f'(p)$.

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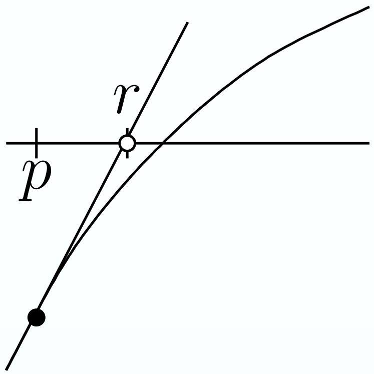

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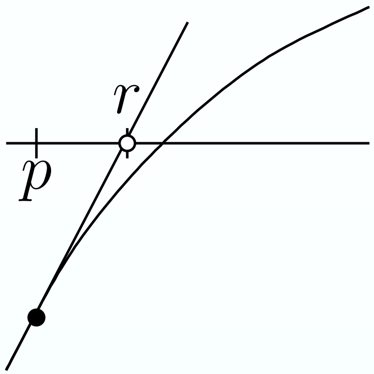

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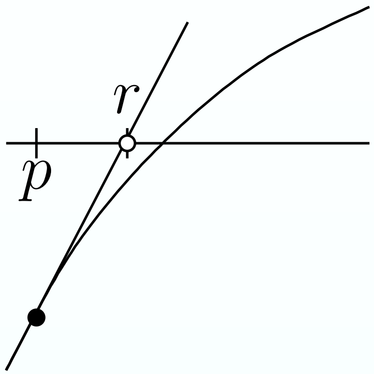

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$$\boxed{p_{n+1} = p_n - \frac{f(p_n)}{f'(p_n)}.}$$

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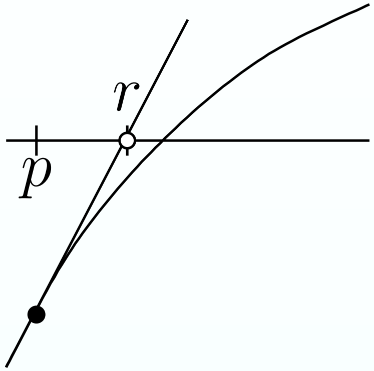

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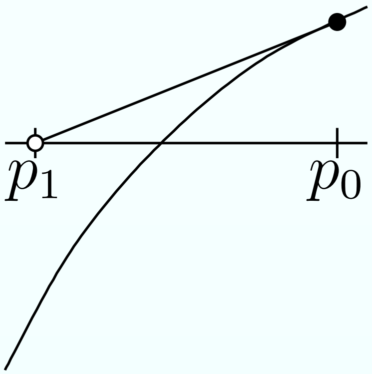

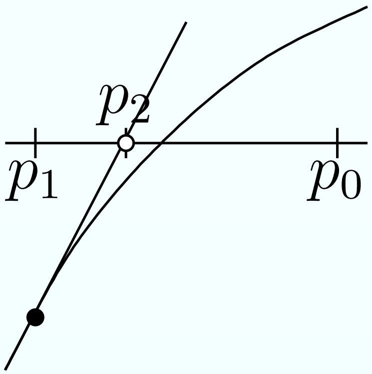

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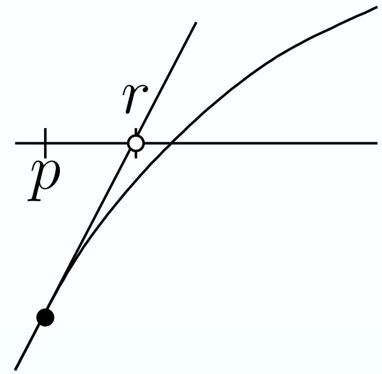

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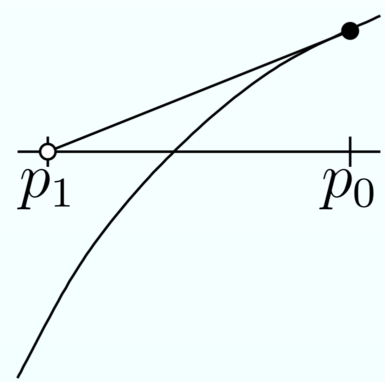

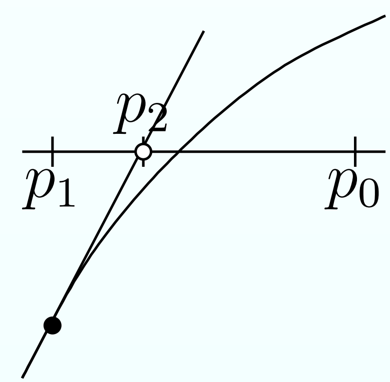

Stopping heuristic As for the secant method, stop when $|p_n - p_{n-1}| < \epsilon$.

Newton-Raphson method

Example Solve $f(x) = x^2 - 2 = 0$ to an accuracy of 0.01.

Newton-Raphson method

Example Solve $f(x) = x^2 - 2 = 0$ to an accuracy of 0.01.

Derivative $f'(x) = 2x$. Start with $p_0 = 1$. Work to 4 decimal places.

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$$p_1 = p_0 - \frac{f(p_0)}{f'(p_0)}$$

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$$p_1 = p_0 - \frac{f(p_0)}{f'(p_0)}$$

$$p_0 = 1.0000$$

$$f(p_0) = 1.0000^2 - 2 = -1.0000;$$

$$f'(p_0) = 2 \times 1.0000 = 2.0000.$$

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\begin{aligned}
p_1 &= p_0 - \frac{f(p_0)}{f'(p_0)} = 1.0000 - \frac{-1.0000}{2.0000} \\
&= 1.5000
\end{aligned}
$$

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Error estimate

$$e_2 := |p_2 - p| \lesssim |p_2 - p_1| = 0.083 > 0.01$$

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Error estimate

$$e_2 := |p_2 - p| \lesssim |p_2 - p_1| = 0.083 > 0.01$$

Need another step!

$$\begin{aligned} p_3 &= p_2 - \frac{f(p_2)}{f'(p_2)} = 1.4167 - \frac{0.0069}{2.8333} \\ &= 1.4167 - 0.0025 = 1.4142. \end{aligned}$$

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Solution $\sqrt{2} \approx p_3 = 1.4142\,(4\,\text{dp}) = 1.41\,(2\,\text{dp})$.

Rounding effects

Rounding effects There is usually a small difference between rounded and exact computation.

For $p_1 = 1.5$, the *exact* value of $p_2 = \frac{17}{12} = 1\frac{5}{12} = 1.41\dot{6} = 1.4167\,(4\,\text{dp})$

Using exact arithmetic, find $p_3 = \frac{577}{408} = 1\frac{169}{408} = 1.41421568\cdots$.

Taking $p_2 = 1.4167$, using rounded arithmetic to 4 decimal places:

$$f(p_2) = f(1.4167) = 1.4167^2 - 2 \overset{4\,\text{dp}}{=} 2.0070 - 2 = 0.0070.$$
$$f'(p_2) = f'(1.4167) = 2 \times 1.4167 - 2.8334.$$

$$p_3 = p_2 - \frac{f(p_2)}{f'(p_2)} = 1.4167 - \frac{0.0070}{2.8334} \overset{4\,\text{dp}}{=} 1.4167 - 0.0025 = 1.4142.$$

In this case, rounding the exact value of p_3 gives the value computed using rounded arithmetic!

This is fairly common in iterative methods:

In iterative methods, rounding errors in early steps can be compensated for by using higher precision in later steps!

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Error decays quadratically; *very* fast.

Comparison of methods

Reliability

+ The bisection method always works.
– The Newton-Raphson method and the secant method may cycle or diverge.

Requirements

+ The bisection and secant methods only require function values.
– The Newton-Raphson method requires the derivative of the function.

Efficiency

– The bisection method converges only linearly, $\epsilon_{n+1} \sim \frac{1}{2}\epsilon_n$
+ The Newton-Raphson method converges superlinearly at rate $\epsilon_{n+1} \sim C\epsilon_n^2$, the secant method $\epsilon_{n+1} \sim C\epsilon_n^{1.6}$.
– Per evaluation of f or f', the Newton-Raphson method is only $O(\epsilon^{1.4})$, slower than the secant method $O(\epsilon^{1.6})$.

Parametrised equations (Non-examinable)

Problem Solve $f(x, y) = 0$ for y in terms of x at points $(x_0, \ldots, x_n)$.

Equivalently, solve $f_a(x) = 0$ for x in terms of the parameter a.

Solution

1. Solve $f(x_0, y) = 0$ using the Newton-Raphson method (or the secant method) with arbitrary starting y to find y_0.

2. Successively solve $f(x_i, y) = 0$ to find y_i, using the solution y_{i-1} for x_{i-1} to *hot-start* the method.

Parametrised equations (Non-examinable)

Solve $f(x, y) = \cos(x) - x + e^x y + y^3 = 0$ for y in terms of x.

Implementation

```
f=@(x,y)cos(x)-x+exp(x)*y+y*y*y;
dyf=@(x,y)exp(x)+3*y*y;
xmin=-4; xmax=+6;
h=0.1; tol=1e-8;
N=round((xmax-xmin)/h);
xs=linspace(xmin,xmax,N+1); ys=xs*NaN;
y=0;
for i=0:N,
    x=xs(i+1); yp=-inf;
    while abs(y-yp)>tol,
        yn=y-f(x,y)/dyf(x,y);
        yp=y; y=yn;
    end;
    ys(i+1)=y;
end;
plot(xs,ys)
```

Systems of equations (Non-examinable)

Systems of nonlinear equations Find a root of $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$.

Newton-Raphson method Generalises directly:

$$\mathbf{p}_{n+1} = \mathbf{p}_n - \mathrm{D}\mathbf{f}(\mathbf{p}_n)^{-1}\mathbf{f}(\mathbf{p}_n).$$

Secant method Generalises to the *simplex method*.

Brent's method (Non-examinable)

Problem The secant method and the Newton-Raphson method do not always converge!

Description Aim to keep *bracketing* properties of the bisection method with the fast convergence of the secant method.

Idea If a secant step does not sufficiently reduce the size of the bracketing interval, use bisection.

Efficiency Don't allow successive bisections.