Numerical Methods in Physics

Numerische Methoden in der Physik, 515.421.

Instructor: Ass. Prof. Dr. Lilia Boeri
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Email Address: l.boeri@tugraz.at

Room: TDK Seminarraum **Time:** 8:30-10 a.m.

Exercises: Computer Room, PH EG 004 F

http://itp.tugraz.at/LV/boeri/NUM_METH/index.html
(Lecture slides, Script, Exercises, etc).

Script:

- For this lecture, I will follow the script of Prof. H. Sormann,

(*Numerische Methoden in der Physik, 515.421*).

You can get a copy (**in German**) at the OH Referat, or at the following web address (pdf):

http://itp.tugraz.at/LV/boeri/NUM_METH/script.html

- I have translated in **English** the parts which are relevant to this lecture (and exercises).

You can get a copy **of the English translation** at the following web address (pdf, updated every week):

http://itp.tugraz.at/LV/boeri/NUM_METH/script_e.html

- Another useful reference is: *R.W. Hamming, Numerical Methods for Scientists and Engineers, Dover Books (in English).*

TOPICS (this year):

- **Chapter 1: Introduction.**
- **Chapter 2: Numerical methods for the solution of linear inhomogeneous systems.**
- Chapter 3: Interpolation of point sets.
- **Chapter 4: Least-Squares Approximation.**
- **Chapter 5: Numerical solution of transcendental equations.**
- Chapter 6: Numerical Integration.
- Chapter 7: Eigenvalues and Eigenvectors of real matrices.
- **Chapter 8: Numerical Methods for the solution of ordinary differential equations: initial value problems.**
- Chapter 9: Numerical Methods for the solution of ordinary differential equations: marginal value problems.

Important !

First Lecture: 1st October 2013.
Last Lecture: 21st January 2014.
Exams: The oral exam can be taken starting on 1st of February 2014 (by appointment).
If somebody has followed the lecture from prof. Sormann in the previous years and would like to take the exam with him please make an appointment with him before the end of the Semester.

First Exercise Class: 1st October 2013.
Last Exercise Class (Last Abgabetermin**):** 21st January 2014.
Exams: The last available date for the presentation of the exercises is the **10th of March 2014. We will accept no exercises after this date.**
If you have not registered yet please tell us NOW!

Important (2):

If you don't have a user account on the TU server, please contact your lecturer (Boeri, Heil, Kapper).

1st Group:	**10:00-11:30**	Lilia Boeri
2nd Group:	**11:30-13:00**	Gernot Kapper
3rd Group:	**13:00-14:30**	Gernot Kapper
4th Group:	**14:30-16:00**	Cristoph Heil

You should have received an email with your group.
If not, please let us know!

Group (1): 10-11:30

Gruppe 1

Nr.	Nachname	Vorname	Mat.Nr.
1	Achtsnit	Tobias	1130687
2	Adam	Manuel	1030270
3	Bodlos	Wolfgang Rao	1131156
4	Braunstingl	Michael	0330830
5	Cesnik	Stefan	1131172
6	Dörschlag	Sarah	1131346
7	Etzlinger	Lukas	1030543
8	Falthansl-Scheinec	Paul	1031841
9	Frantz	Florentine Valerie	1031053
10	Fuchs	Arthur	1130421
11	Glatz	Matthias	0831197
12	Gößler	Markus	1130844
13	Grasserbauer	Jakob	1131331
14	Greil	Georg	1130673
15	Gruberbauer	Andreas	1030874
16	Ranftl	Sascha	1030670
17	Muralter	Fabian	1131191
18*	Hallama	Bernhard	9913937

Group (2): 11:30-13:00

Gruppe 2

Nr.	Nachname	Vorname	Mat.Nr.
1	Heim	Pascal	1130870
2	Hengge	Elisabeth	1130921
3	Henögl	Elias Michael	0931157
4	Hofer	Alexander David	1130210
5	Hofer	Sebastian	1130204
6	Hörmann	Lukas	1130254
7	Jeindl	Andreas	1131189
8	Kaltenegger	Martin	1031169
9	Kappe	Florian	1131316
10	Koroschitz	Tobias	1031288
11	Kozeschnik	Markus	0932012
12	Krainer	Alexander Michae	1130700
13	Lageder	Benjamin	1131627
14	Lainscsek	Xenia	1131233
15	List	Hans	1031472
16	Meier	Thomas	1131397
17	Stindl	Robert	1130957
18	Skrilec	Filip	1130536
19	Pranter	Alexander	931114
20*	Hollomey	Marc	1031185

Group (3): 13:00-14:30

Gruppe 3

Nr.	Nachname	Vorname	Mat.Nr.
1	Freitag	Anna	1030759
2	Messner	Roman	1131131
3	Meszaros	Robert	1130698
4	Millner	Gerfried Dankwar	0931550
5	Neuhold	Manuel	1031287
6	Pfleger	Alexander Julian	1131137
7	Pilat	Florian	1131145
8	Pilz	Julian	1130527
9	Pliemon	Thomas	1018275
10	Postl	Andreas	0731097
11	Rastjoo	Seyedeh Sanaz	1131774
12	Riemer	Christoph	1030526
13	Rosmann	Patrick	1131993
14	Ruckhofer	Adrian	1130414
15	Salzmann	Paul Karl	1013828
16	Scherbela	Michael	1130975
17	Vötter	Rene	1030375
18*	Schlick	Christopher	1130206

Group (4): 14:30-16:00

Gruppe 4

Nr.	Nachname	Vorname	Mat.Nr.
1	Schicho	Philipp	1110068
2	Schönhuber	Benedikt	1130636
3	Schwendt	Mathias	1031305
4	Seeber	Florian	1130904
5	Sejkora	Christoph	1131265
6	Simenc	Thomas	0130881
7	Sorgmann	Benjamin Josef	1031170
8	Strasser	Anna Theresa	0912757
9	Tazreiter	Martin Josef	1130735
10	Thaler	Bernhard	1131253
11	Theiler	Andreas	1131297
12	Tumphart	Stephan	1058315
13	Uhde	Navid	1031201
14	Wappis	Erich	0031093
15	Weißenbacher	Fabian	1130667
16	Winkler	Christian	1230797
17	Berger	Richard Klaus	1031520
18*	Ramsauer	Bernhard	1130877
19*	Thommesen	Kristian	831441
20*	Fritzenwallner	Julia	931269

Important (3):

IMPORTANT: Please note that, according to a new TU regulation, all students who attend the first two classes of an exercise class and then “drop out” of the course, will fail (5) the exercise class. We will enforce this rule for all students who present the first exercise and “disappear” afterwards!

SCRIPT

Chapter 1: Introduction

Outline (today):

- Definitions and basic concepts: algorithm, machine precision, roundoff.
- Errors: absolute and relative error; sources of error.
- Input Errors: ill-conditioned problems.
- Sources of errors in the algorithms: methodological errors.
- Practical Examples of the interplay of methodological and roundoff errors:

    - Function Evaluation: how to avoid subtractive cancellation.

    - Numerical Differentiation: optimal stepsize.

    - Taylor series and continued fraction.

    - Recursive Algorithms.

Definitions

Important Concepts

Numerical Mathematics: *"Numerical Mathematics concerns the solution of **mathematical problems** using **numerical calculations**. This term indicates a finite sequence of basic mathematical operations, such as addition, subtraction, multiplication and divisions, using **finite-digits algebra**".*

Algorithm: *"A finite number of precise instructions, which require specific input data and, executed in a given sequence, determine the final solution".*

Error: *"The results of computer calculations are (with a few exceptions) subject to errors, i.e. they do not coincide exactly with the "true" solution of the problem".*

Errors:

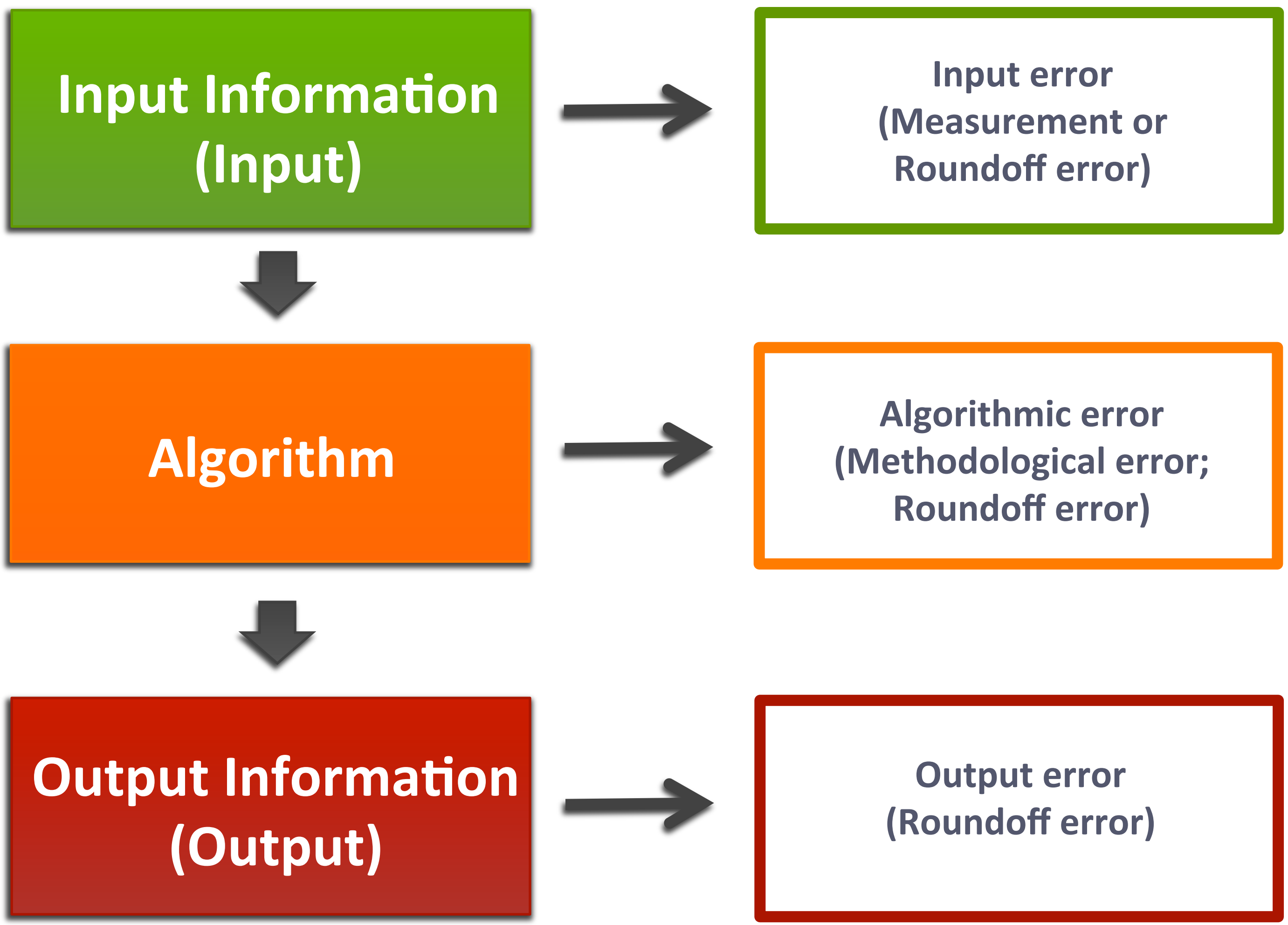
Absolute and relative error.

$x, \bar{x}$ Real and Approximate value of x

Absolute Error: $\varepsilon_a = x - \bar{x}$

Relative Error: $\varepsilon_r = \frac{\varepsilon_a}{\bar{x}} = \frac{x - \bar{x}}{\bar{x}}$ → *More meaningful*

	x	$\bar{x}$	ϵ_a	ϵ_r
(a)	0.1	0.09	0.01	≈ 0.1
(b)	1000.0	999.99	0.01	≈ 0.00001


Input Information
(Input)
Input error
(Measurement or
Roundoff error)
Algorithm
Algorithmic error
(Methodological error;
Roundoff error)
Output Information
(Output)
Output error
(Roundoff error)

Machine Precision

Definition

Machine Precision: The machine precision is the smallest positive number τ for which:

$$1 + \tau > 1$$

The smaller τ, the higher the **accuracy** of the machine.

	Bytes	τ	Number sign. digits
C-float	4	$1.19 \cdot 10^{-7}$	7
C-double	8	$2.22 \cdot 10^{-16}$	16
F90-real	4	$1.19 \cdot 10^{-7}$	7
F90-double prec.	8	$2.22 \cdot 10^{-16}$	16
Pascal-single	4	$1.19 \cdot 10^{-7}$	7
Pascal-real	6	$1.82 \cdot 10^{-12}$	12
Pascal-double	8	$2.22 \cdot 10^{-16}$	16
Pascal-extended	10	$1.08 \cdot 10^{-19}$	19

How to determine τ in practice?

Structure chart 1 — Determination of the parameter τ

```
tau:=1.0
wold:=1.0
    tau:=tau/2.0
    wnew:=wold + tau
wnew=wold
print: 2*tau
```

```
// C-PROGRAM FOR THE CALCULATION OF MACHINE PRECISION

#include <iostream.h>

void main()
{
  float tau,wold,wnew;

  tau=1.0;
  walt=1.0;
  do {
    tau/=2.0;
    wnew=wold+tau;
  } while (wnew != wold);
  cout <<"TAU = "<<2*tau<<"\n";
}
```

Roundoff Error

Definition

Roundoff Error: Roundoff Errors are unavoidable, and derive from the fact that in a computer only a limited number of bits is available to represent a real number (or better, its *mantissa*).

Scientific (floating point) Notation: A real number is expressed using a significand and an exponent. The mantissa represents the significant digits of the number.

$$1.2345 = \underbrace{12345}_{\text{Mantissa}} \times 10^{\overbrace{-4}^{\text{Exponent}}}$$

The **mantissa** contains the **significant digits** of the number.

Significant Digits:

```
Calculation "by Hand":              Computer (7 sign. digits):

   123456.789                          0.1234568E+06
+        9.876543                   +  0.9876543E+01
----------------                    ----------------
   123466.665543                       0.1234667E+06
```

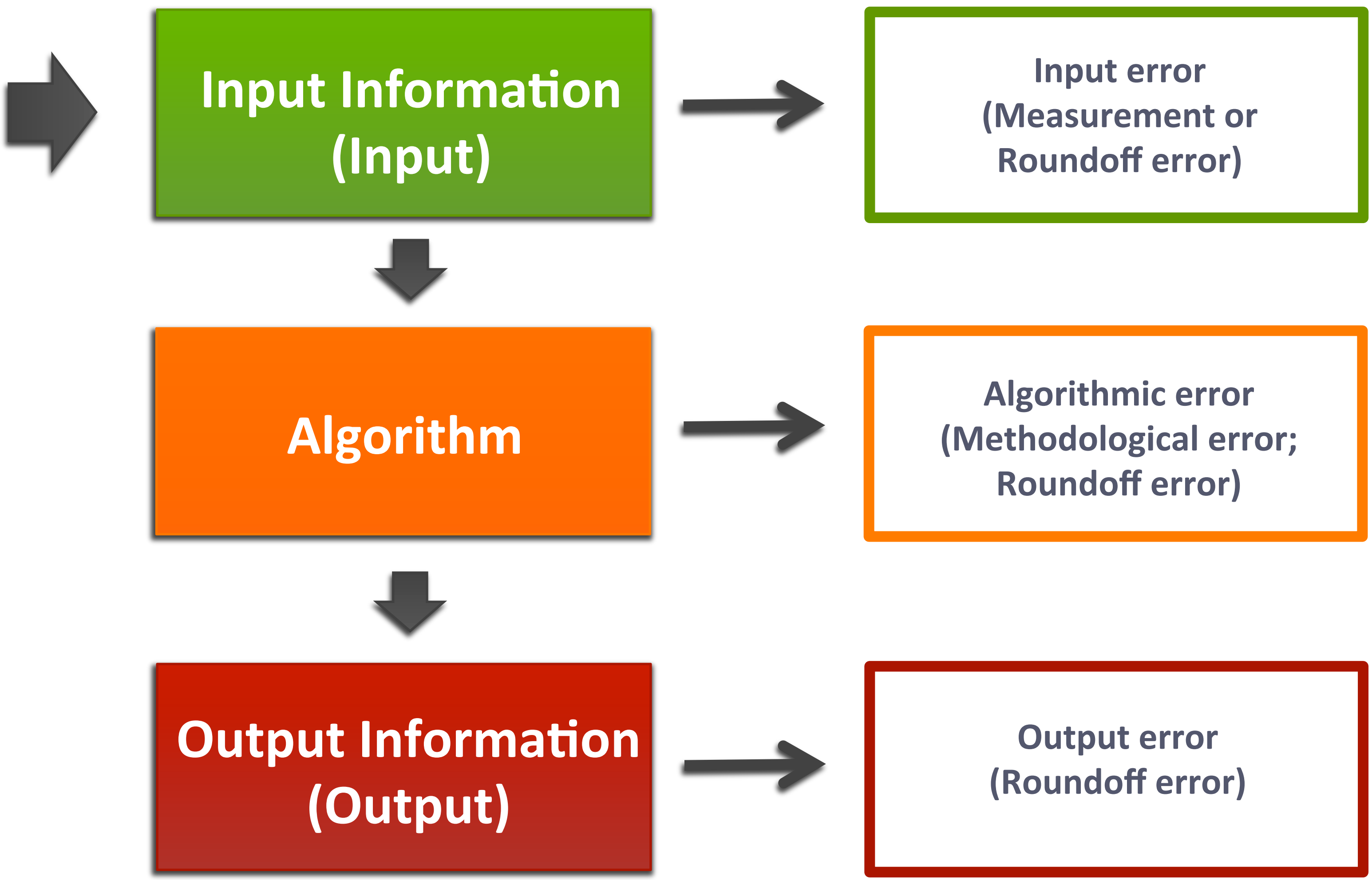
Roundoff in practice:

Structure chart 2 — Demonstration of the effect of roundoff errors

```
value:=0.1
sum:=0.0
i=1(1)50
    sum:=sum + value
print: sum
```

Result: 4.9999998

$$0.1_{10}=0.000110011001100..._2$$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Output error
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Input Errors

Definition

Input Errors: Input errors (i.e. inherent errors) are uncertainities in the input data with which the computer performs the calculations. These uncertainities can have several origins, such as experimental (measuring) errors, or roundoff error.

Ill-conditioned systems: are those systems for which the results of a calculation are strongly influenced by errors in the input data. In this case, the results of a calculation can be completely meaningless!

Let's see a simple example…

2x2 linear set of equations:

$$\begin{cases} x + 5.0y = 17.0 \\ 1.5x + 7.501y = a \end{cases}$$

$$\begin{cases} x = 17.0 - 5.0y \\ 1.5(17.0 - 5.0y) + 7.501y = a \end{cases}$$

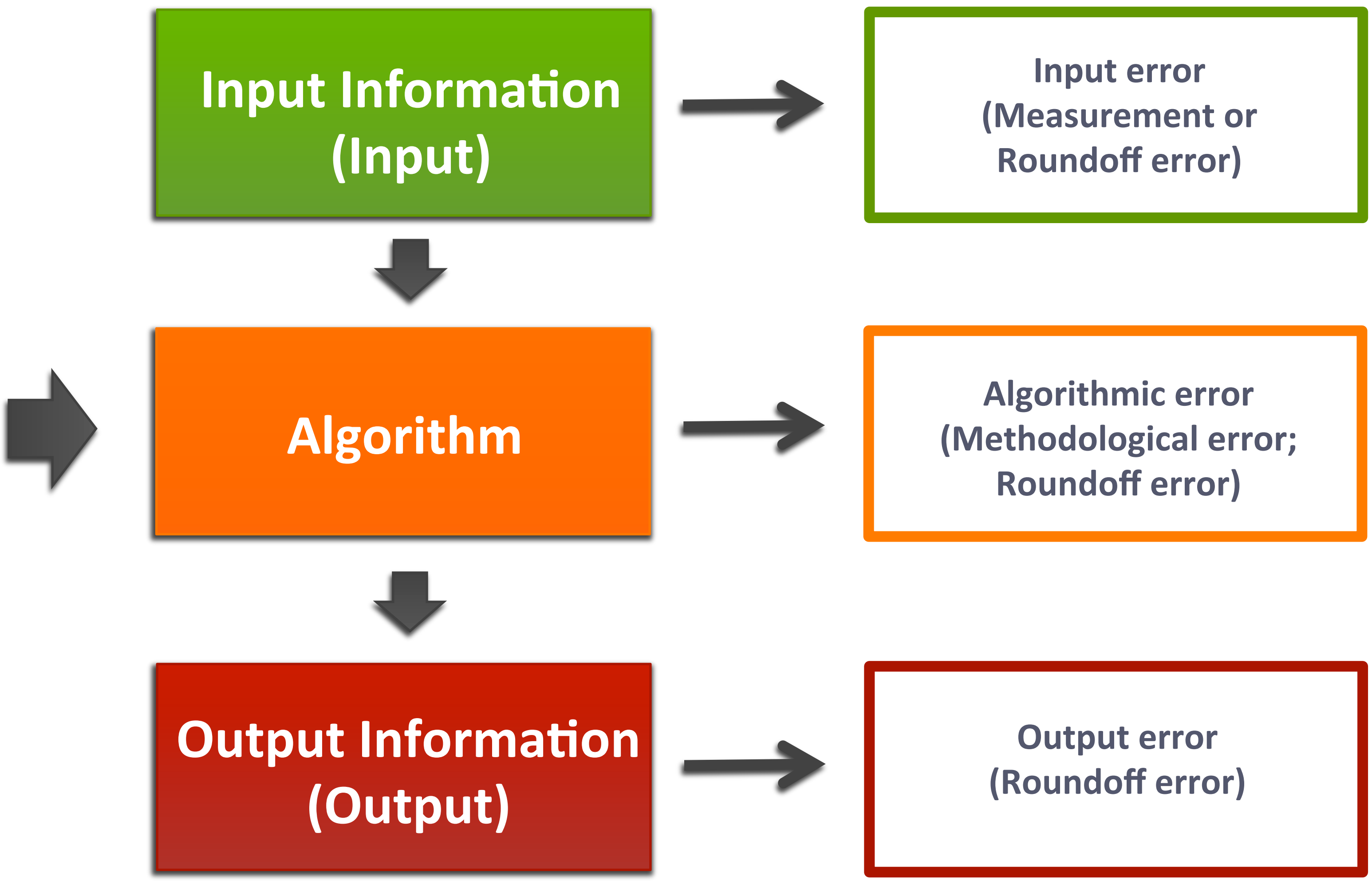
$$\begin{cases} x = 17.0 - 5.0y \\ y = \dfrac{a - 25.5}{0.001} \end{cases}$$

Exact Solution

What happens if there is an ***uncertainity*** on *a*?

$$a = 25.503 \pm 0.001$$

a	x	y
25.503	2.	3.
25.502	7.	2.
25.504	-3.	4.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Output error
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Algorithmic Errors

Definition

Algorithmic Errors: are errors that occur during the evaluation of the calculation specification. The causes are **roundoff** or **methodological** errors.

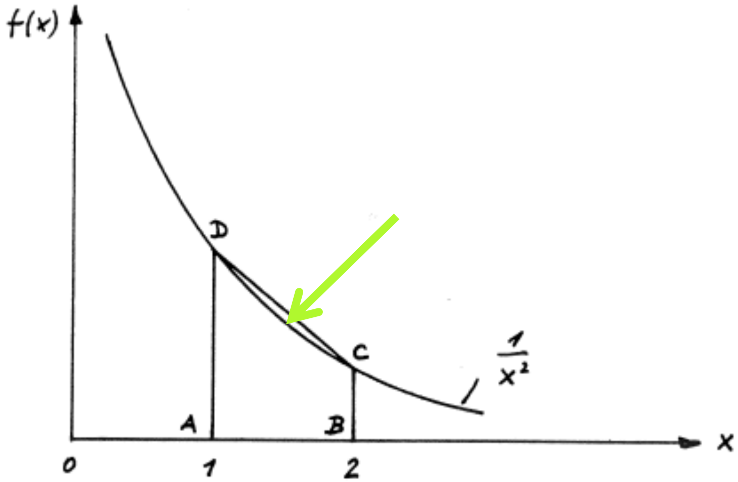
Methodological Errors: occur when the original mathematical problem is replaced by a simplified problem.

- **Example:**

$$I=\int_{x=1}^{2}\frac{dx}{x^2}=-\frac{1}{x}\bigg|_{x=1}^{x=2}=1-\frac{1}{2}=0.5$$

Exact Solution

Approximate Solution: trapezoidal formula.



$$I = \frac{f(1)+f(2)}{2}\Delta x = (\frac{1}{4}+1)\cdot\frac{1}{2} = \frac{5}{8}$$

$$\varepsilon_a = 0.5 - 0.625 = -0.125$$

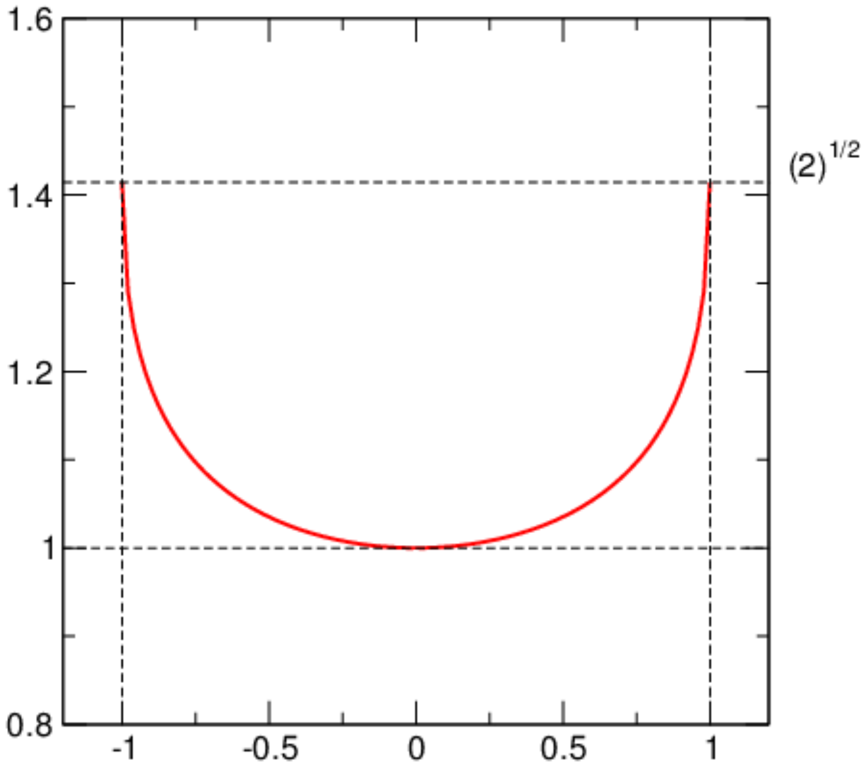
Absolute error introduced by the trapezoidal formula (*methodological error*).

Practical Examples

Characteristic examples of methodological/roundoff errors

Example: Function Evaluation: Interplay of roundoff and methodological errors.

$$F(x) = \frac{\sqrt{1+x} - \sqrt{1-x}}{x}$$

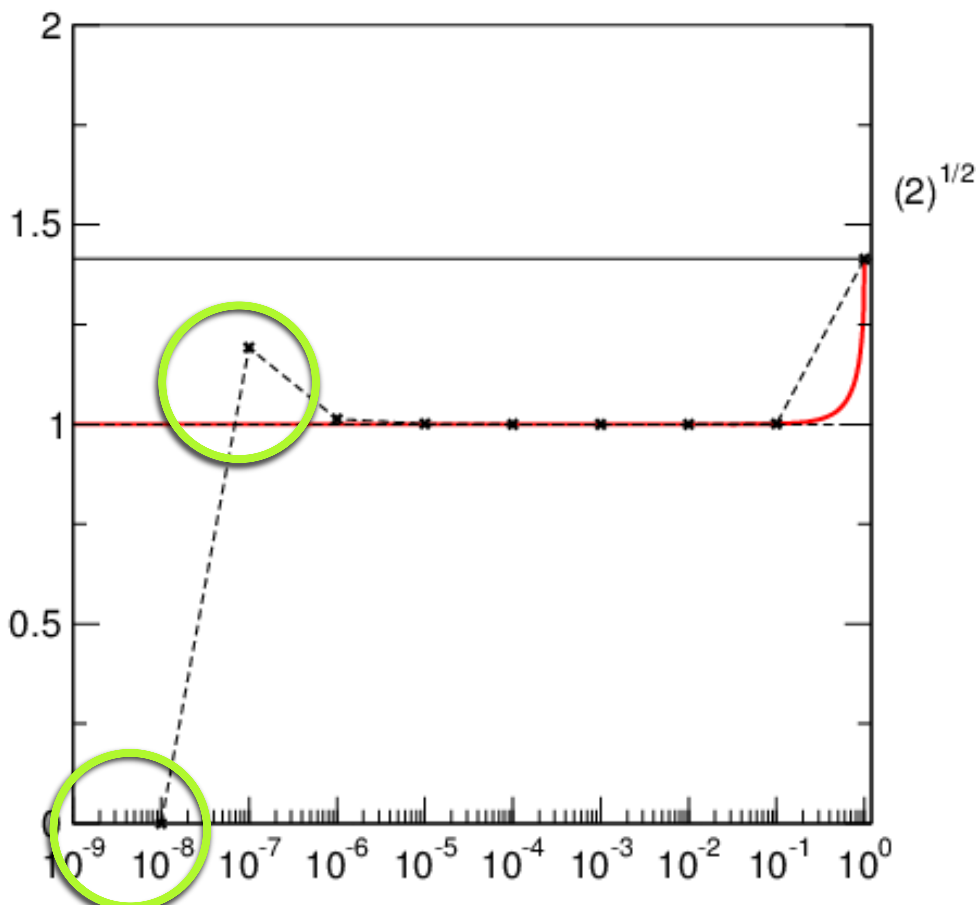


Exact result:

$$F(1) = F(-1) = \sqrt{2}$$

$$F(0) = 1$$

$$F(x) = \frac{\sqrt{1+x} - \sqrt{1-x}}{x}$$



Numerical Solution:

Straightforward Evaluation of F(x): The results are **problematic** for **small** values of ***x***.

$$F_{ex}(0) = 1 \rightarrow F_{num}(0) = 0$$

$$F(x) = \frac{\sqrt{1+x} - \sqrt{1-x}}{x}$$

What is the problem for **small *x***?

For **small *x***: $\sqrt{1+x} \approx \sqrt{1-x}$

Subtractive cancellation of roundoff error + divide by "*almost zero*"!

(crazy oscillations)

For "really" **small *x*** *(x≈τ)*:

Machine Precision

$$\sqrt{1+x} = \sqrt{1-x} \Rightarrow F(0) = 0!$$

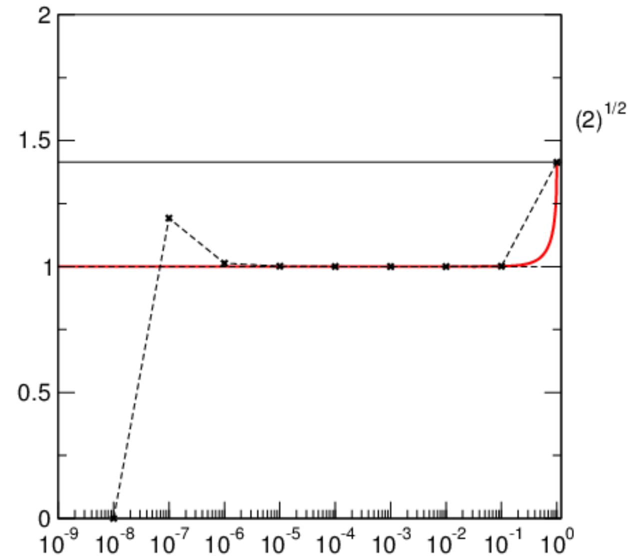
(wrong limit)

Solution: rewrite F(x) in an equivalent form, which is not affected by subtractive cancellation.

$$F1(x) \equiv F(x) = \frac{\sqrt{1+x}-\sqrt{1-x}}{x} \cdot \frac{(\sqrt{1+x}+\sqrt{1-x})}{(\sqrt{1+x}+\sqrt{1-x})} = \frac{2}{(\sqrt{1+x}+\sqrt{1-x})}$$

Tab.1.1: Numerical evaluation of F(x) and F1(x).

x	F	F1
10^0	$0.1414214E+01$	$0.1414214E+01$
10^{-1}	$0.1001256E+01$	$0.1001256E+01$
10^{-2}	$0.1000013E+01$	$0.1000013E+01$
10^{-3}	$0.1000041E+01$	$0.1000000E+01$
10^{-4}	$0.1000153E+01$	$0.1000000E+01$
10^{-5}	$0.1001357E+01$	$0.1000000E+01$
10^{-6}	$0.1013279E+01$	$0.1000000E+01$
10^{-7}	$0.1192093E+01$	$0.1000000E+01$
10^{-8}	$0.0000000E+01$	$0.1000000E+01$



Another Example: Second-order equations.

$$ax^2 + bx + c = 0$$

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

$$x_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

If *a* and *c* are small, of **subtractive cancellation** for x_1 ($b>0$) and x_2 ($b<0$).

Reformulation:

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \times \frac{-b - \sqrt{b^2 - 4ac}}{-b - \sqrt{b^2 - 4ac}} =$$

$$= \frac{b^2 - b^2 + 4a^2c^2}{2a(-b - \sqrt{b^2 - 4ac})} = \frac{2c}{-b - \sqrt{b^2 - 4ac}}$$

No subtractive cancellation!

Alternative Formulas:

$$x_1 = \frac{q}{a}$$

$$x_2 = \frac{c}{q}$$

$$q = -\frac{1}{2}\left[b + \operatorname{sgn}(b)\sqrt{b^2 - 4ac}\right]$$

Example: <u>Numerical Differentiation</u>: Interplay of roundoff and methodological errors.

$$\left.\frac{d}{dx}f(x)\right|_{x=x_0} \approx \frac{f(x+h)-f(x)}{h}$$

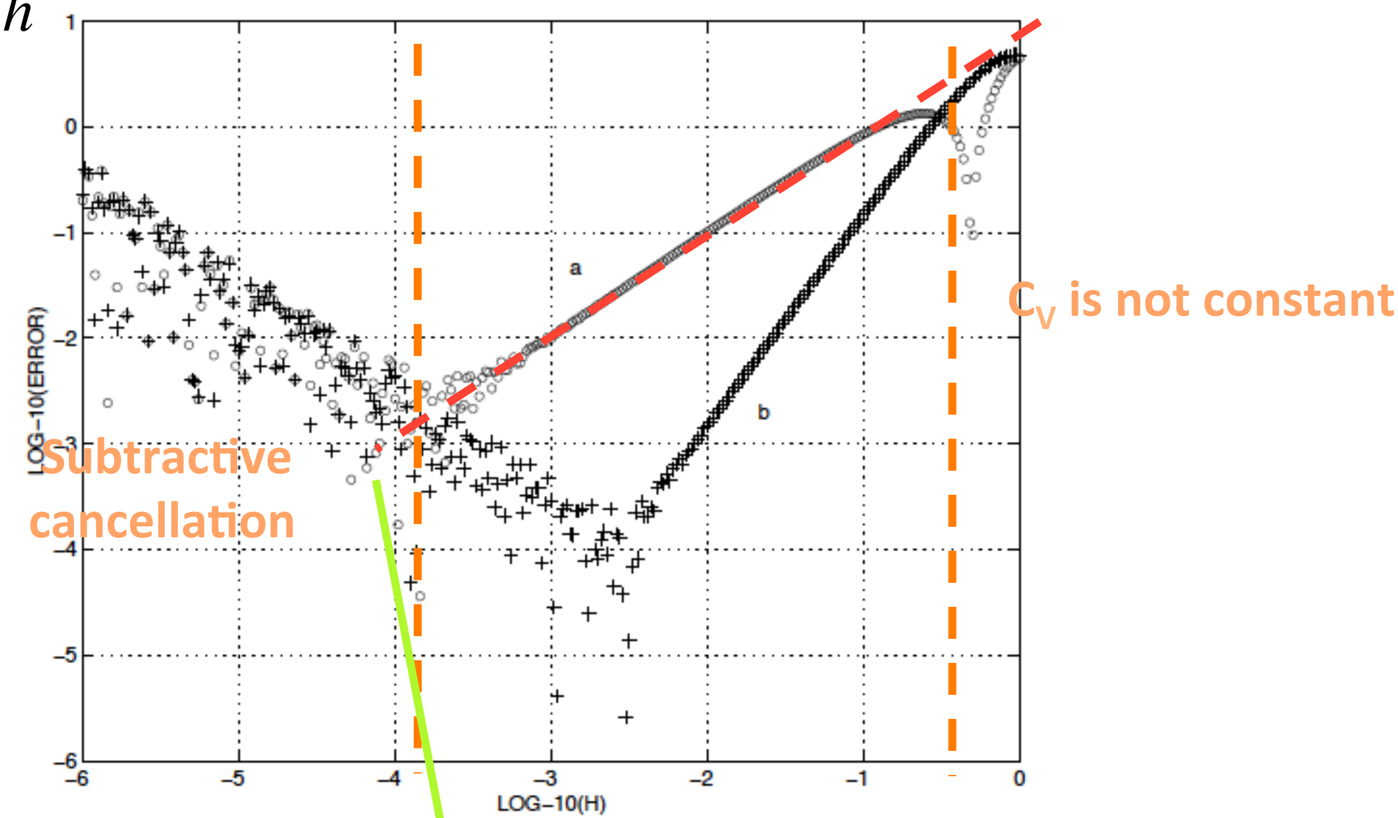
- Differential ratio
- *h*: stepsize (finite increment)

Using a finite stepsize introduces a *methodological* error ε_V, which gets smaller and smaller with decreasing h.
In practice, the behaviour is **roughly linear** with h:

$$\varepsilon_V(h) = C_V(h)\cdot h$$

$$C_V(h) \approx C_V$$

$$\varepsilon_V(h) = C_V(h) \cdot h$$



$$\log \varepsilon_V = \log C_V + \log h$$

There is an **optimal value** of the stepsize (h_{opt})

How to improve the methodological error?

1) Increase precision (single/float->double).
2) Use an improved formula:

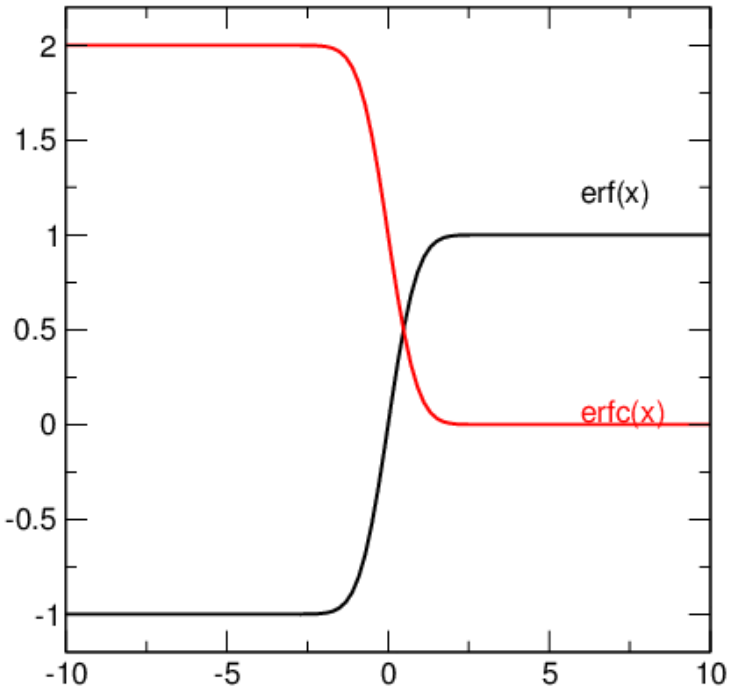
$$\frac{d}{dx} f(x)\Big|_{x=x_0} \approx \frac{f(x_0+h)-f(x_0-h)}{2h}$$

In many cases the methodological error is larger than the roundoff error, therefore it is possible to assess (limit) the total error of the calculation.

Taylor Series

Example: Complementary error function.

$$erfc(x) = 1 - erf(x)$$



Error Function: The error function is is related to the cumulative distribution Φ, **the integral of the standard normal distribution** by:

$$\Phi(x)=1/2+1/2erf(x/\sqrt{2})$$

The error function, evaluated at x/(σ√2)} for positive x values, gives the probability that a measurement, under the influence of normally distributed errors with standard deviation σ, has a distance less than x from the mean value.This function is used in statistics to predict behavior of any sample with respect to the population mean.

Complementary Error Function: Taylor Series expansion.

$$erfc(x) = 1 - \frac{2}{\pi}\int_{z=0}^{x} dz e^{-z^2} = 1 - \frac{2}{\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n+1}}{n!(2n+1)}$$

$$erfc(x) = 1 - \frac{2}{\sqrt{\pi}}\sum_{n=0}^{n\max} a_n, \qquad a_n = \frac{(-1)^n x^{2n+1}}{n!(2n+1)}$$

Recursion Formula:

$$a_n = \left[-\frac{x^2(2n-1)}{n(2n+1)}\right]a_{n-1}, n \geq 1; \qquad a_0 = x$$

The **truncation error** (truncating the series at $n=n_{max}$) is smaller than a_{nmax+1}.
It is possible to evaluate the series **up to machine precision**! (no methodological error!)

Structure Chart — Evaluation of a Taylor series

```
x:= .....

n:=0
sumnew:=x
a:=x

    n:=n+1
    taylor:=sumnew
    a:= -x*x*(2*n-1)/n/(2*n+1) * a
    sumnew:=sumnew+a

sumnew=taylor

print: x, taylor
```

Tab.1.2: Evaluation of the function erfc(x) through a Taylor series and a continuous fraction. All results are given in half-exponential form with 7 digits for the mantissa. The exponent E indicates a calculation in simple precision, the exponent D a calculation in double precision.

x	Taylor series $\epsilon_V = 0$	Cont. Fract. 31 Terms	Cont. Fract. 61 Terms
0.01	0.9887166E+00	0.1261318E+02	0.9042203E+01
	0.9887166D+00	0.1261318D+02	0.9042202D+01
0.1	0.8875371E+00	0.1401417E+01	0.1131721E+01
	0.8875371D+00	0.1401417D+01	0.1131721D+01
0.5	0.4795001E+00	0.4802107E+00	0.4795305E+00
	0.4795001D+00	0.4802107D+00	0.4795305D+00
1.	0.1572992E+00	0.1572995E+00	0.1572992E+00
	0.1572992D+00	0.1572995D+00	0.1572992D+00
2.	0.4677685E-02	0.4677735E-02	0.4677735E-02
	0.4677735D-02	0.4677735D-02	0.4677735D-02
3.	0.2991446E-04	0.2209050E-04	0.2209050E-04
	0.2209050D-04	0.2209050D-04	0.2209050D-04
4.	0.2364931E-02	0.1541726E-07	0.1541726E-07
	0.1544033D-07	0.1541726D-07	0.1541726D-07
5.	0.4645361E+02	0.1537460E-11	0.1537460E-11
	0.5458862D-07	0.1537460D-11	0.1537460D-11

Alternative method: Continued Fraction

$$\operatorname{erfc}(z) = \frac{z}{\sqrt{\pi}} e^{-z^2} \cfrac{a_1}{z^2 + \cfrac{a_2}{1 + \cfrac{a_3}{z^2 + \cfrac{a_4}{1 + \cdots}}}} \qquad a_1 = 1, \quad a_m = \frac{m-1}{2}, \quad m \geq 2.$$

Advantage: works also for large values of the argument x.
Disadvantage: difficult to evaluate a priori the accuracy; cannot add terms to the formula (to increase accuracy have to restart evaluation from scratch).

Tab.1.2: Evaluation of the function erfc(x) through a Taylor series and a continuous fraction. All results are given in half-exponential form with 7 digits for the mantissa. The exponent E indicates a calculation in simple precision, the exponent D a calculation in double precision.

x	Taylor series $\epsilon_V = 0$	Cont. Fract. 31 Terms	Cont. Fract. 61 Terms
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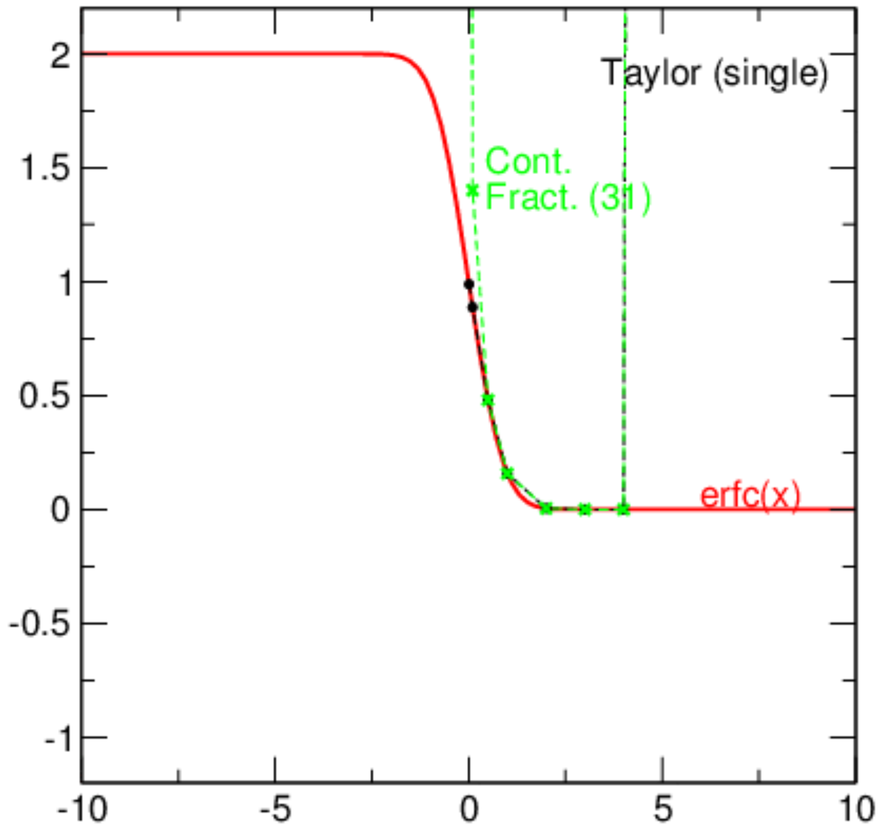
	0.9887166D+00	0.1261318D+02	0.9042202D+01
0.1	0.8875371E+00	0.1401417E+01	0.1131721E+01
	0.8875371D+00	0.1401417D+01	0.1131721D+01
0.5	0.4795001E+00	0.4802107E+00	0.4795305E+00
	0.4795001D+00	0.4802107D+00	0.4795305D+00
1.	0.1572992E+00	0.1572995E+00	0.1572992E+00
	0.1572992D+00	0.1572995D+00	0.1572992D+00
2.	0.4677685E-02	0.4677735E-02	0.4677735E-02
	0.4677735D-02	0.4677735D-02	0.4677735D-02
3.	0.2991446E-04	0.2209050E-04	0.2209050E-04
	0.2209050D-04	0.2209050D-04	0.2209050D-04
4.	0.2364931E-02	0.1541726E-07	0.1541726E-07
	0.1544033D-07	0.1541726D-07	0.1541726D-07
5.	0.4645361E+02	0.1537460E-11	0.1537460E-11
	0.5458862D-07	0.1537460D-11	0.1537460D-11

Methodological Error

Comparison of different methods:



Recursion: A recursive algorithm is defined by a *recursion formula*:

$$y_n = a \cdot y_{n-1} + b \cdot y_{n-2}$$

Stability: An algorithm is defined stable (or unstable) when the error with respect to the exact result at the nth step of the calculation decreases (or increases) in the following steps.

Summary:

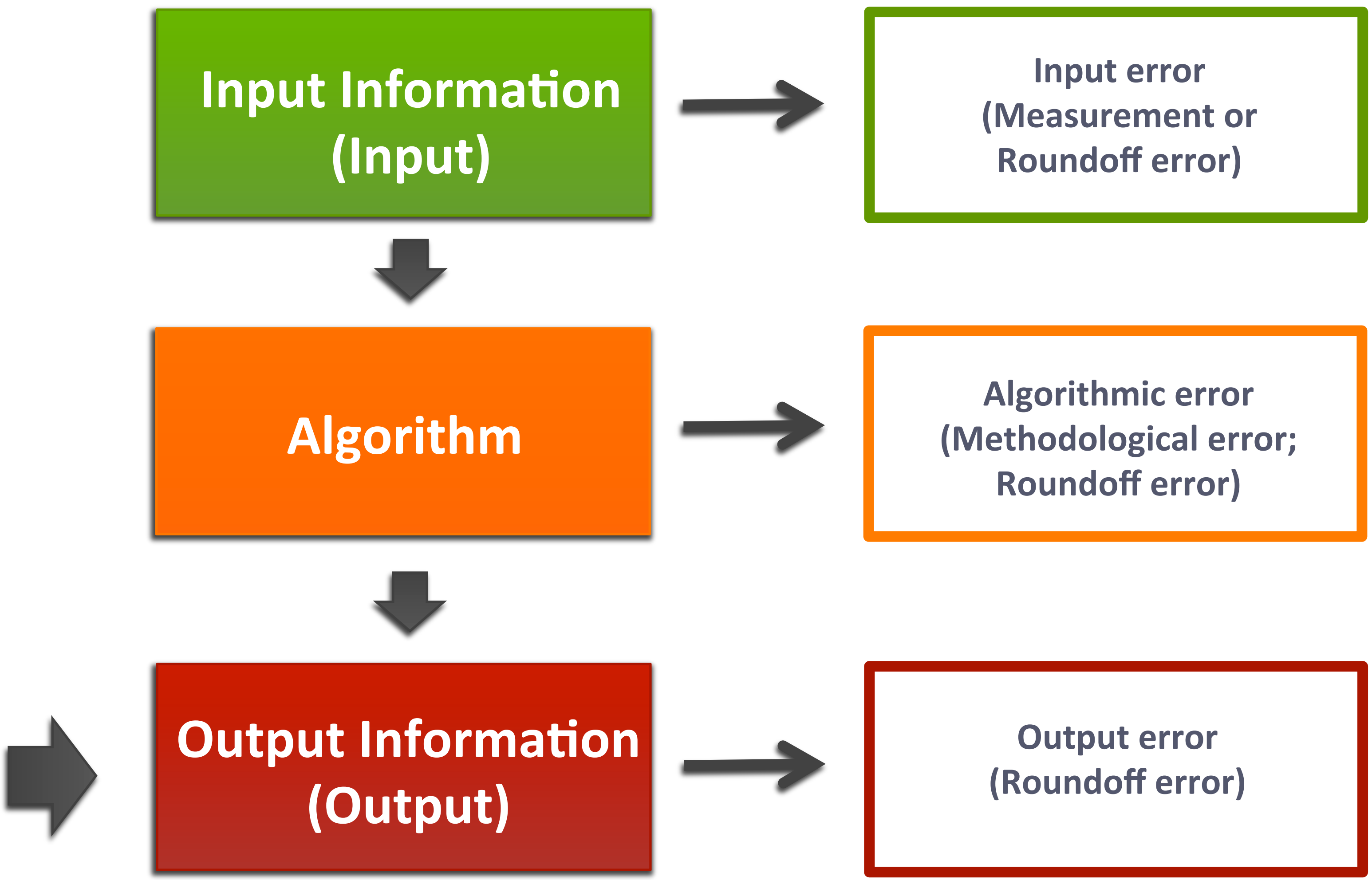
- Definitions and basic concepts: algorithm, machine precision, roundoff.
- Errors: absolute and relative error; sources of error.
- Input Errors: ill-conditioned problems.
- Sources of errors in the algorithms: methodological errors.
- Practical Examples of the interplay of methodological and roundoff errors:

    - Function Evaluation: how to avoid subtractive cancellation.

    - Numerical Differentiation: optimal stepsize.

    - Taylor series and continued fraction.

    - Recursive Algorithms.


Input Information
(Input)
Input error
(Measurement or
Roundoff error)
Algorithm
Algorithmic error
(Methodological error;
Roundoff error)
Output Information
(Output)
Output error
(Roundoff error)