Numerical methods

Numerical analysis is the study of algorithms
for the problems of continuous mathematics.

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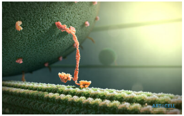


Elementary theory of uncertainties

Numerical solutions are always approximate

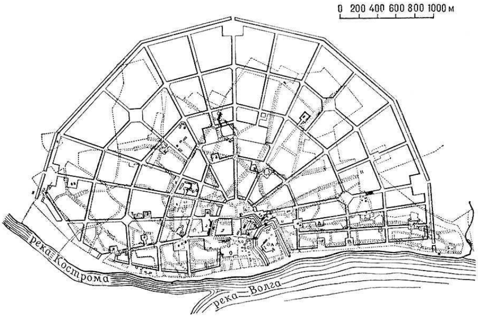
1. Mathematical models are approximate
2. Input data are approximate, may contain e.g., measurement uncertainties
3. Mathematical methods are approximate
4. Computer arithmetics is inexact (more below)

We need to be able to quantify the degree of approximation, and design algorithms to control and minimize what we can (esp. 3 and 4 above.)

Example: area on a map

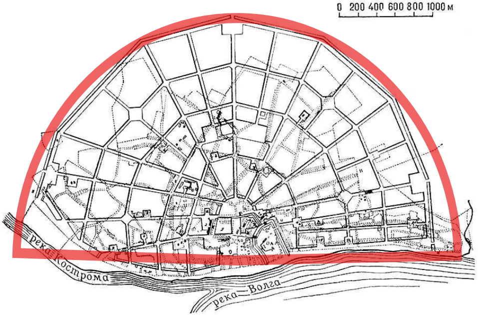
City of Kostroma, 1781-84

Here's the map. Find the area of the city.



Example: area on a map

City of Kostroma, 1781-84



$$R \approx 2.4\,\mathrm{km}$$

$$S = \pi R^2/2 \approx 9.2\,\mathrm{km}^2$$

The model is approximate (the surface is flat; the map is drawn to scale). The method is approximate (the city is approximated by a semicircle). The input data is only measured approximately. The calculation uses finite precision.

Approximate numbers. Uncertainties.

Let S be an (unknown) exact number. Let S^* be a known value which approximates S.

The absolute uncertainty of S^* (absolute error, абсолютная погрешность, абсолютная ошибка) is defined as

$$\Delta S \equiv |S - S^*| \; .$$

Likewise,

$$\delta S \equiv \frac{\Delta S}{S} \equiv \frac{|S - S^*|}{S} \; .$$

is the relative error (относительная погрешность) of S^*.

Approximate numbers. Uncertainties.

Since the exact value S is typically not known, we are mostly interested in the upper limits for the uncertainties,

$$|S - S^*| \leqslant \overline{\Delta} S$$

and

$$\frac{|S - S^*|}{S} \leqslant \bar{\delta} S$$

To lighten the notation, we typically omit the overlines and simply write ΔS and δS to mean the upper limits of the uncertainties.

Fixed-point representation of real numbers. Significant figures

Let an approximate number a^* is given as a finite decimal fraction

$$a^* = \beta_n \beta_{n-1} \dots \beta_1 \beta_0 . \alpha_1 \alpha_2 \dots \alpha_p$$

Significant figures (значащие цифры): all α-s and β-s except for leading zeros, if any.

For example: 0.42 has two s.f.; 0.4200 has four s.f

Common abbreviations: “Significant figures” $\rightarrow$ ***sig figs*** or ***s.f.***

A significant figure is ***correct*** (верная значащая цифра) iff the absolute uncertainty of a^* is less than a 1 in the corresponding decimal place.

Significant figures and uncertainties

The number of correct significant figures in a^* is directly related to the relative uncertainty of a^*:

if a^* has N correct significant figures, then $\delta a \sim 10^{-N}$

We always only write out correct sig figs. A number without uncertainty means all sig figs are correct.

Example: "Rounding to N s.f.": π to 3 s.f. is 3.14; π to 6 s.f. is 3.14159

Note: rounding to a correct number of s.f. is what tells a human from a machine. A computer may output 16 digits; it's our job to round to a correct number of s.f.

Significant figures and uncertainties

When writing out uncertainties:

- Always round uncertainties to 1 or 2 s.f.

$$1.234 \pm 0.002 \qquad \text{(good)}$$
$$1.234000 \pm 0.001895 \qquad \text{(bad)}$$

- Use consistent s.f. for both value and its uncertainty.

$$1.23 \pm 0.02 \qquad \text{(good)}$$
$$1.234567 \pm 0.02 \qquad \text{(bad)}$$
$$1.23 \pm 0.00005 \qquad \text{(bad)}$$

Arithmetics with approximate numbers. Propagation of uncertainty.

Consider two unknown quantities, a and b. Suppose that we know approximations a^* and b^*, with uncertainties Δa and Δb.

The (upper limit of the) uncertainty of $a + b$ is

$$\Delta(a+b) \leqslant \Delta a + \Delta b$$

Indeed,

$$\begin{aligned} \Delta(a+b) &= |(a+b) - (a^* + b^*)| \\ &= |(a - a^*) + (b - b^*)| \\ &\leqslant |a - a^*| + |b - b^*| \\ &\leqslant \Delta a + \Delta b \end{aligned}$$

Arithmetics with approximate numbers. Propagation of uncertainty.

Consider two unknown quantities, a and b. Suppose that we know approximations a^* and b^*, with uncertainties Δa and Δb.

The (upper limit of the) uncertainty of $a - b$ is

$$\Delta(a-b) \leqslant \Delta a + \Delta b$$

Indeed,

$$\begin{aligned} \Delta(a-b) &= |(a-b) - (a^* - b^*)| \\ &= |(a - a^*) - (b - b^*)| \\ &\leqslant \Delta a + \Delta b \end{aligned}$$

Notice the plus sign in the r.h.s.

Catastrophic cancellation

Let $a = 101$ and $b = 100$ are both known to 3 s.f.

The difference,

$$a - b = 1$$

is only known to 1 s.f.

$\Longrightarrow$ ***avoid (i) subtraction of close numbers, (ii) divisions by small numbers***

Example: Try computing

$$\frac{1}{\sqrt{x+1} - \sqrt{x}} = \sqrt{x+1} + \sqrt{x}$$

for $x \gg 1$ (do try it!)

Propagation of uncertainty in nonlinear operations

Let $f(x)$ be a differentiable function of its scalar argument. Suppose x is only known with an absolute uncertainty Δx. What is the uncertainty of $y = f(x)$?

Assuming $\Delta x \ll |x|$, expand $f(x + \Delta x)$ into the Taylor series:

$$f(x + \Delta x) = f(x) + f'(x)\,\Delta x + \cdots .$$

Therefore,

$$\Delta y \leqslant |f'(x)|\,\Delta x \ ,$$

and the relative uncertainty is ($\Delta x = x\,\delta x$)

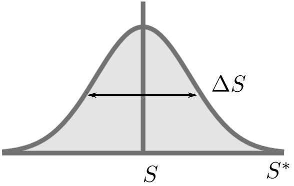
$$\delta y \leqslant \left| \frac{f'(x)\,x}{f(x)} \right| \delta x$$

Sidetrack: An alternative, stochastic view of uncertainties.

The difference between the true value S and measured approximation S^* is due to ***random noise***.

The distribution of measured values

Multiple repeated measurements produce different values of S^*.



The assumption is that the distribution of S^* is ***Gaussian***, centered at the true value S. The uncertainty, ΔS, is then the width of this Gaussian distribution.

The sum of two independent Gaussian variables is also Gaussian, with the width

$$\Delta(a+b) = \sqrt{(\Delta a)^2 + (\Delta b)^2}$$