Mathematics for Informatics

Numerical mathematics
(lecture 9 of 12)

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Outline

- Introduction to numerical mathematics
- Computer arithmetics
- Conditioning and stability of an algorithm
- Direct and iterative methods
- Systems of linear equations

Numerical mathematics

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The following mathematical problems are often involved:

1. solution of systems of linear equations,
2. solution of differential equations,
3. calculation of integrals,
4. evaluations of function values,
5. estimation of errors in calculations,
6. . . .

Typically, a computer calculation is involved.

From the history

- Error in the Patriot missile system

$$(0.1)_{10} = (0.000110011001100110011001100110011...)_2$$

- Explosion of the Ariane 5 rocket
  conversion from a 64-bit floating point number to a 16-bit signed integer

- . . .

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This does not mean that approximation methods do not work. In the vast majority of cases they work well, but it is important to know how reliable they are.

Category of errors

We will use different **approximations** to design the algorithm. We will therefore make various kind of mistakes, which can be divided according to their origin:

1. errors in the **model**: the mathematical model to solve the problem is somehow simplified.
2. errors in the **data**: data often come from measurements that do not have absolute accuracy.
3. errors in the **algorithm**: we don't have to have an algorithm that finds the exact solution in a finite number of steps.
4. **rounding** errors: errors occur during the calculation itself (e.g., during arithmetic operations).

Apart from data errors, we will give examples of all other kinds of errors. We start with rounding errors, which are given by the fact that the algorithm need a computer to do the hard work.

Representation with floating point

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For non-integers, one can use the **scientific notation**. In the binary base a number x is represented as

$$x = \pm\, m \cdot 2^e.$$

m - **mantissa/significand** having a fixed number of digits / fixed length; these digits are also called **significant digits**.

e - **exponent** having a fixed number of digits / fixed length.

IEEE-754

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precision	length of m	d = length of e	b
`binary32` / single precision	23	8	127
`binary64` / double precision	52	11	1023
`binary128` / quadruple precision	112	15	16383

- if $e = 2^d - 1$ and $m \neq 0$, then $x = \texttt{NaN}$ (Not a Number)
- if $e = 2^d - 1$ and $m = 0$ and $s = 0$, then $x = +\texttt{Inf}$
- if $e = 2^d - 1$ and $m = 0$ and $s = 1$, then $x = -\texttt{Inf}$
- if $0 < e < 2^d - 1$, then $x = (-1)^s \cdot (1.m)_2 \cdot 2^{e-b}$ (so-called **normalized numbers**)
- if $e = 0$ and $m \neq 0$, then $x = (-1)^s \cdot (0.m)_2 \cdot 2^{-b+1}$ (so-called **subnormal/unnormalized numbers**)
- if $e = 0$ and $m = 0$ and $s = 0$, then $x = 0$
- if $e = 0$ and $m = 0$ and $s = 1$, then $x = -0$

Machine numbers (1/3)

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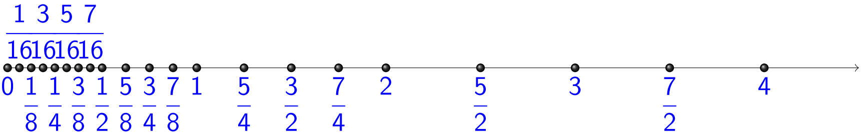
Example: take m of length 2 bits, e of length 3 bits, and $b = 3$.

We obtain the following set of numbers (we consider only positive elements)

$$\left\{0, \frac{1}{16}, \frac{1}{8}, \frac{3}{16}, \frac{1}{4}, \frac{5}{16}, \frac{3}{8}, \frac{7}{16}, \frac{1}{2}, \frac{5}{8}, \frac{3}{4}, \frac{7}{8}, 1, \frac{5}{4}, \frac{3}{2}, \frac{7}{4}, 2, \frac{5}{2}, 3, \frac{7}{2}, 4, 5, 6, 7, 8, 10, 12, 14\right\}$$

Subnormal numbers are in brown.



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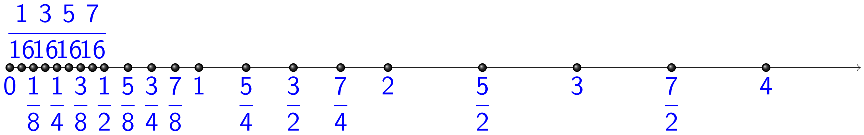

The set of all machine numbers with a given precision has little in common with the set of real numbers. It resembles more to a finite subset of integers.

Machine numbers (2/3)

Denote the set of machine numbers by F.

The set F has the largest and the smallest positive elements as follows:

precision	max. no.	min. pos. normalized	min. pos. subnormal
single	$(2-2^{-23})\cdot 2^{127}$ $\approx 3.4\cdot 10^{38}$	2^{-126} $\approx 1.2\cdot 10^{-38}$	$2^{-126-23}=2^{-149}$ $\approx 1.4\cdot 10^{-45}$
double	$(2-2^{-52})\cdot 2^{1023}$ $\approx 1.8\cdot 10^{308}$	2^{-1022} $\approx 2.2\cdot 10^{-308}$	$2^{-1022-52}=2^{-1074}$ $\approx 4.9\cdot 10^{324}$

Machine numbers (3/3)

F is characterized by the **machine epsilon** ϵ_F, which is the difference between 1.0 and the smallest number in F larger than 1.

For single precision we have $\epsilon_F = 2^{-23}$, for double 2^{-52}.

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Proposition

The distance between any two neighboring normalized numbers in F *is at least* $\frac{\epsilon_F}{2}$ *and at most* ϵ_F*.*

Representation of real numbers (1/3)

Let $fl : \mathbb{R} \to F$ be the mapping which assigns to any $x \in \mathbb{R}$ the closest machine number.

The "closest" is given by the method chosen: rounding ("ties to even"), chopping (rounding towards 0),. . .

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When trying to represent a number which is out of the representable range, an **overflow** or **underflow** is returned.

Definition

Let a number α be an approximate value of a number a.

- *The* ***absolute error*** *is the value $|\alpha - a|$.*
- *For $a \neq 0$, the* ***relative error*** *is $\dfrac{|\alpha - a|}{|a|}$.*

Representation of real numbers (2/3)

In single precision, suppose that a number $x \in \mathbb{R}$ lies in the normalized range, i.e.,

$$x = q \cdot 2^{\ell}, \quad \text{where } 1 \leq q < 2 \text{ and } -126 \leq \ell \leq 127.$$

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Let's round towards 0, i.e., chop off bits which do not fit into the significand (for positive numbers).

$$\text{If} \quad x = (1.b_1 b_2 b_3 b_3 \ldots)_2 \cdot 2^{\ell} \qquad \text{then} \quad fl(x) = (1.b_1 b_2 \ldots b_{23}) \cdot 2^{\ell}.$$

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The absolute error and the absolute errors are respectively:

$$|x - fl(x)| \leq 2^{-23+\ell} \qquad \text{and} \qquad \frac{|x - fl(x)|}{|x|} \leq \frac{2^{-23+\ell}}{q \cdot 2^{\ell}} \leq 2^{-23}.$$

Representation of real numbers (3/3)

The threshold of relative error is called the **unit roundoff error** and is denoted by $\mathbf{u}$. Thus, in the single precision with chopping we have $\mathbf{u} = 2^{-23}$.

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Proposition

Let $x \in \mathbb{R}$ be greater than the smallest normalized number of F and smaller than the greatest normalized number of F. We have

$$fl(x) = x(1+\delta), \quad \textit{where} \; |\delta| \leq \mathbf{u},$$

Arithmetic operations - error

Proposition

Let $x, y \in F$ and $\odot$ be the operation of addition, multiplication or division. If there is no overflow or underflow, then we have

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In general: If we operate with more numbers, it is better to start with the smallest ones.

Arithmetic operations - a demonstration

Let $f : \mathbb{R}^2 \mapsto \mathbb{R}$ be a mapping given by

$$f(x,y) = 333.75y^6 + x^2\left(11x^2y^2 - y^6 - 121y^4 - 2\right) + 5.5y^8 + \frac{x}{2y}.$$

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Let us evaluate $f(77617, 33096)$:

SageMath (precision 23 bits)	1.17260
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The exact solution is $-\frac{54767}{66192} \approx -0.827396$.

[S. M. Rump: *Algorithms for verified inclusions - theory and practice*, ..., 1988]

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Big problems can be caused by the so-called **cancellation**.

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We want to evaluate $x - \sin(x)$ for $x = \frac{1}{15}$.

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Let us calculate the relative error.

Loss of significant digits (2/3)

$$\frac{\left|\frac{1}{15}-\sin\left(\frac{1}{15}\right)-fl\Big(fl\left(\frac{1}{15}\right)-\sin\left(fl\left(\frac{1}{15}\right)\right)\Big)\right|}{\left|\frac{1}{15}-\sin\left(\frac{1}{15}\right)\right|}\approx 1.4\cdot 10^{-7}.$$

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That is a lot in comparison to

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Proposition

*Let x and y be normalized machine numbers and $x > y > 0$. If $2^{-p}\leq 1-\dfrac{y}{x}\leq 2^{-q}$ for some positive integers p and q, then **at most** p and **at least** q significant binary bits are lost when performing the operation $x-y$.*

Loss of significant digits (3/3)

Cancellation can be avoided by using the following techniques:

- rationalizing the problem, i.e., using rational numbers and avoiding the subtraction in floating points arithmetics,
- using series expansions (such as Taylor series),
- using other identities,. . .

Errors - conclusion

Origins of errors:

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A few final notes:

- increased precision may not lead to a more precise result,
- cancellation can be useful - it may cancel rounding errors,
- few operations with small numbers do not imply a small error.

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There are some alternatives:

- Exact arithmetics: $\mathbb{Z}$, $\mathbb{Q}$ or $GF(p)$ (it is not always possible or suitable).
- Interval arithmetics (we work with intervals instead of points). (`IEEE 1788-2015`).
- Unum.

Example: system of linear equations (1/2)

Consider two systems of linear equations with 2 unknowns:

$$\begin{pmatrix} 1 & 1/2 \\ 1/2 & 1/3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3/2 \\ 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 1/5 \\ 1/5 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3/2 \\ 1 \end{pmatrix}.$$

The solutions are

$$(x,y)^T = (0,3)^T \quad \text{and} \quad (x,y)^T = (85/52, -35/52)^T \approx (1.6346, -0.67308)^T.$$

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Let us try to simulate an error on the input, or during a calculation, by changing the right side to $\begin{pmatrix} 3/2 \\ 5/6 \end{pmatrix}$.

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The solutions change to

$$(x,y)^T = (1,1)^T \quad \text{and} \quad (x,y)^T = (125/78, -20/39)^T \approx (1.6026, -0.51282)^T.$$

Example: system of linear equations (2/2)

The change in the right side was

$$\begin{pmatrix} 3/2 \\ 1 \end{pmatrix} - \begin{pmatrix} 3/2 \\ 5/6 \end{pmatrix} = \begin{pmatrix} 0 \\ 1/6 \end{pmatrix},$$

a vector of Euclidean length $1/6$ (the relative error is 0.09).

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The change in the solution of **the first equation** was

$$\begin{pmatrix} 0 \\ 3 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \end{pmatrix}$$

(the relative error is 0.75) and the one in the solution of **the second equation**

$$\begin{pmatrix} 85/52 \\ -35/52 \end{pmatrix} - \begin{pmatrix} 125/78 \\ -20/39 \end{pmatrix} = \begin{pmatrix} 5/156 \\ -25/156 \end{pmatrix}$$

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Why is it that the first system is more sensitive to this change? Why are the two relative errors so different?

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$$\begin{tikzcd}
d + \Delta d \arrow[r, "V"] & V^*(d) \\
d \arrow[u, "\Delta d"] \arrow[r, "V"'] \arrow[ur, dashed, "V^*"'] & V(d) \arrow[u, "\Delta v"']
\end{tikzcd}$$

Forward and backward error

Let V be a numerical algorithm whose theoretical (accurate) output is denoted by $V^*(d)$ where d is the input.

The result in the finite arithmetic is denoted $V(d)$. Furthermore, denote the so-called **forward error** by $\Delta v := V^*(d) - V(d)$.

The least (in a norm) number Δd such that $V(d + \Delta d) = V^*(d)$ is the **backward error**.

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\end{tikzcd}$$

If for all considerable inputs d the backward error is relatively small, we say that the algorithm is **backward stable**. “Small” depends again on the context.

Conditioning

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$$C_r = \lim_{\varepsilon \to 0^+} \sup_{\substack{d+\delta d \in D \\ \|\delta d\| \leq \varepsilon}} \frac{\dfrac{\|V(d+\delta d) - V(d)\|}{\|V(d)\|}}{\dfrac{\|\delta d\|}{\|d\|}},$$

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where D is the domain of V.

If $C_r \approx 1$, then we say that the problem is **well-conditioned**.
If it is large, we say the problem is **ill-conditioned**.

Direct methods

A **direct method** calculates a solution of a problem in finitely many steps such that in absolute theoretical precision in gives the exact solution.

Idea of iterative methods

Iterative methods look for approximate solutions to mathematical problems by constructing a sequence of approximate solutions:

$$x_0,\ x_1,\ x_2,\ \dots$$

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Every following (approximate) solution is derived from the previous:

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for $k > 0$ and some mapping T.

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If T is the same for all k, the method is called **stationary**.

System of linear equations

We want to solve a system of n linear equations. We write the system in matrix representation

$$Ax = b,$$

where $A \in \mathbb{R}^{n,n}$ is regular and $b \in \mathbb{R}^{n,1}$.

This is often a partial subproblem of a larger problem.

Norm - reminder

A **norm** on a vector space V is a mapping $\|\cdot\| : V \mapsto \mathbb{R}_0^+$ which satisfies

1. $\|x\| = 0 \quad \Rightarrow \quad x = 0$,
2. $\|\alpha x\| = |\alpha| \cdot \|x\|$,
3. $\|x + y\| \leq \|x\| + \|y\|$ (triangle inequality),

for all $x, y \in V$ and all scalars α.

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On $\mathbb{R}^n$ (or $\mathbb{C}^n$) the most used norm is probably the **Euclidean norm**:

$$\|x\| = \left(\sum_{i=1}^{n} x_i^2 \right)^{\frac{1}{2}},$$

where $x = (x_1, x_2 \ldots, x_n) \in \mathbb{R}^n$.

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Other commonly used norms include

- $\|x\|_\infty = \max\big\{|x_i| \colon i \in \{1, \ldots, n\}\big\}$ maximum norm,
- $\|x\|_1 = \sum_{i=1}^{n} |x_i|$ taxicab or L_1 norm.

Matrix norm

Given a vector norm $\|\cdot\|$, we define the **induced matrix norm** of the matrix $A \in \mathbb{C}^{n,n}$ as follows

$$\|A\| = \sup\left\{\|Ax\| : x \in \mathbb{C}^{n,1} \text{ and } \|x\| = 1\right\}.$$

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Such norm satisfies

- $\|I\| = 1$,
- $\|Ax\| \leq \|A\| \cdot \|x\|$ (norm consistency),
- $\|AB\| \leq \|A\| \cdot \|B\|$.

Conditioning of the problem (1/2)

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Finally,

$$\frac{\|\delta x\|}{\|x\|} \leq \|A\| \cdot \|A^{-1}\| \frac{\|\delta b\|}{\|b\|},$$

Conditioning of the problem (2/2)

$$\frac{\|\delta x\|}{\|x\|} \leq \left(\|A\| \cdot \|A^{-1}\|\right) \frac{\|\delta b\|}{\|b\|}$$

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Of course, the condition number depends on the chosen norm.

Example of two sets of linear equations revisited

Let us revisit the example we saw earlier:

$$A = \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1/3 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 1 & 1/5 \\ 1/5 & -1 \end{pmatrix},$$

The inverses are

$$A^{-1} = \begin{pmatrix} 4 & -6 \\ -6 & 12 \end{pmatrix} \quad \text{and} \quad B^{-1} \approx \begin{pmatrix} 0.961538 & 0.192308 \\ 0.192308 & -0.961538 \end{pmatrix},$$

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To calculate the condition number $\kappa(A) = \|A\| \cdot \|A^{-1}\|$ we use the norm $\|A\|_\infty$:

$$\kappa(A) = \|A\|_\infty \cdot \|A^{-1}\|_\infty = \frac{3}{2} \cdot 18 = 27 \quad \text{and} \quad \kappa(B) = \frac{18}{13} \approx 1.3846056.$$

The problem with the matrix A is significantly more **ill-conditioned** than with the matrix B. This is in accordance with our previous observations.

Basic iterative methods for $Ax = b$

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We choose a regular matrix Q and the following terms will be calculated as

$$Qx_k = (Q - A)x_{k-1} + b$$

for all $k > 0$.

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for all $k > 0$.

The idea: we choose the matrix Q so that the sequence (x_k) converges to some x^*. Then,

$$Qx^* = (Q - A)x^* + b$$

and thus

$$Ax^* = b.$$

Convergence - choice of Q

We use the equality $x_k = Q^{-1}\big((Q-A)x_{k-1}+b\big)$ in

$$\begin{array}{rcl} x_k - x & = & Q^{-1}\big((Q-A)x_{k-1}+b\big) - x \\ & = & (I - Q^{-1}A)x_{k-1} - x + Q^{-1}b \\ & = & (I - Q^{-1}A)x_{k-1} - (I - Q^{-1}A)x \\ & = & (I - Q^{-1}A)(x_{k-1} - x), \end{array}$$

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The vector e_k will be "smaller" than e_{k-1} if W is "small".
"Small" can be determined using norms.

Since $e_k = W^k e_0$, to lower the error at each step we need to have $\lim\limits_{k\to+\infty} W^k = 0$.

Convergence vs. spectral radius

The **Spectral radius** of a matrix M is the number $\rho(M)$ defined as the greatest eigenvalues (in absolute value), i.e.,

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If $M \in \mathbb{C}^{n,n}$, then

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Theorem

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$$\lim_{k \to +\infty} M^k = 0 \quad \Leftrightarrow \quad \rho(M) < 1,$$

Thus, in our case, the method converges **if and only if**

$$\rho(W) < 1,$$

i.e., all the eigenvalues of the matrix $W = I - Q^{-1}A$ are in absolute value less than 1.

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Suppose that M is diagonalizable, i.e., there exists a change of basis P such that $M = PDP^{-1}$, where

$$D = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix},$$

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We have $M^k = PDP^{-1}\,PDP^{-1}\,PDP^{-1}\cdots = PD^kP^{-1}$.

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and $\rho(M) < 1$, i.e., for all i we have $|\lambda_i| < 1$, then $\lim\limits_{k\to+\infty} D^k = 0$.

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Overall $\lim_{k\to+\infty} M^k = P\left(\lim_{k\to+\infty} D^k\right)P^{-1} = 0$.

If M is not diagonalizable, the proof is very similar - the Jordan normal form is used instead of the diagonal matrix.

Speed of convergence of e_k

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The condition of convergence $\rho(W) < 1$ does not imply anything on the speed from the previous estimate.

However, the estimate on the right side is strictly decreasing if $\|W\| < 1$.

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The desired precision is given by the nature of the problem.

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In the case $\|W\| < 1$, we know that the sequence $(\|e_k\|)_k$ is strictly decreasing and we may stop iterating when

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This is impractical since we do not have the exact solution.

In the step k we can calculate the so-called **residue** $Ax_k - b$ and the **convergence criterion** can be set to

$$\|Ax_k - b\| < \varepsilon.$$

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Instead of calculating the residues, one may use a more efficient criterion

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where, supposing $\|W\| < 1$, the last inequality gives

$$\|e_k\| < \frac{\varepsilon}{1 - \|W\|}.$$

Thus, this criterion can be effectively used if $\|W\| < 1$, but not too close to 1.

Finite precision calculations

All ideas so far were made in the theoretical absolute precision.
In a finite precision, the method may not converge even if $\|W\| < 1$ due to rounding errors.

However, an advantage of iterative methods in a finite precision arithmetic is that at each step the rounding errors from the previous step are "forgotten". We start the new iteration with a better approximate solution.

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However, an advantage of iterative methods in a finite precision arithmetic is that at each step the rounding errors from the previous step are "forgotten". We start the new iteration with a better approximate solution.

In finite arithmetic the method can diverge even if the problem is not ill-conditioned.

Thus, in practice, we need another parameter of the method - a maximum number of iterations. If we reach this number of iterations without satisfying a convergence criterion, then the method outputs failure.

Choices of Q

Denote by $a_{i,j}$ the entries of the matrix A and denote

$$L = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ a_{2,1} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ a_{n,1} & \cdots & a_{n,n-1} & 0 \end{pmatrix} \text{ and } D = \begin{pmatrix} a_{1,1} & 0 & \cdots & 0 \\ 0 & a_{2,2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & a_{n,n} \end{pmatrix}.$$

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Denote U so that $A = L + D + U$.

We will mention the following choices of Q:

- Richardson method $Q = I$,
- Jacobi method $Q = D$,
- successive overrelaxation / SOR method $Q = \dfrac{1}{\omega} D + L$.

Richardson method

Set $Q = I$.

The recurrence relation is given by

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The convergence is for a narrow class of matrices: A must be close to I so that

$$\|I - A\| < 1.$$

Jacobi method

Set $Q = D$.

The recurrence relation is given by

$$Dx_k = (D - A)x_{k-1} + b = -(L + U)x_{k-1} + b.$$

Jacobi method

Set $Q = D$.

The recurrence relation is given by

$$Dx_k = (D - A)x_{k-1} + b = -(L + U)x_{k-1} + b.$$

Proposition

If the matrix A is diagonally dominant, then the Jacobi method converges for any choice of x_0.

A matrix is diagonally dominant if, for each row, the sum of the absolute values of all the entries except the one on the diagonal is less than the absolute value of the entry on the diagonal.

SOR method

Set $Q = \frac{1}{\omega} D + L$, where $\omega \in \mathbb{R} \setminus \{0\}$.

The recurrence relation is given by

$$\left(\frac{1}{\omega} D + L\right) x_k = \left(\frac{1}{\omega} D + L - A\right) x_{k-1} + b = \left(\left(-1 + \frac{1}{\omega}\right) D - U\right) x_{k-1} + b.$$

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Proposition

For $0 < \omega < 2$ the SOR method converges if A is symmetric, positive definite and has positive diagonal entries.

The parameter ω is used to speed up the convergence.
The choice $\omega = 1$ is the *Gauss-Seidel* method.

Algorithm

Inputs: matrices A, Q, vector b, precision ε, maximum number of iterations K.

```
1. choose $\widehat{x}_0$ at random
2. for $k$ from $1$ to $K$ do
    2.1 $\widehat{x}_{k+1} = Q^{-1}(Q - A)\widehat{x}_k + Q^{-1}b$
    2.2 if $\|A\widehat{x}_k - b\| < \varepsilon$, **return** $\widehat{x}_k$ (or in general if any convergence criterion is satisfied)
3. **return** “no solution found after $K$ steps”.
```

Demonstration - Jacobi method (1/2)

Let $A = \begin{pmatrix} 2 & 1 \\ 1 & 4 \end{pmatrix}$. $\|I - D^{-1}A\| = \frac{1}{2}$.

We use the Jacobi method to calculate a solution for $b = (3,5)^T$.
The exact solution is $(1,1)^T$.

The convergence criterion used is $\|A\widehat{x}_k - b\| < 10^{-2}$.

k	$\widehat{x}_k$	$\|A\widehat{x}_k - b\|$
0	$(0.5, 1.5)$	1.58113883008
1	$(0.75, 1.125)$	0.450693909433
2	$(0.9375, 1.0625)$	0.197642353761
3	$(0.96875, 1.015625)$	0.0563367386791
4	$(0.9921875, 1.0078125)$	0.0247052942201
5	$(0.99609375, 1.001953125)$	0.00704209233489

Demonstration - Jacobi method (2/2)

...the same problem but with a different $\widehat{x}_0$, which is further from the exact solution.

k	$\widehat{x}_k$	$\|A\widehat{x}_k - b\|$
0	$(-10, 10)$	28.1780056072
1	$(-3.5, 3.75)$	9.01734439844
2	$(-0.375, 2.125)$	3.5222507009
3	$(0.4375, 1.34375)$	1.1271680498
4	$(0.828125, 1.140625)$	0.440281337613
5	$(0.9296875, 1.04296875)$	0.140896006226
6	$(0.978515625, 1.017578125)$	0.0550351672016
7	$(0.9912109375, 1.00537109375)$	0.0176120007782
8	$(0.997314453125, 1.002197265625)$	0.0068793959002