Mathematics for Informatics

Numerical Mathematics 1
(lecture 8 of 12)

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Outline

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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

$$(0.1)_{10} = (0.0001100110011001100110011001100110011...)_2$$

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

- ...

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Representation with floating point

To store a number in computer we usually use the binary number system.

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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.

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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 $x =$ `NaN` (Not a Number)
- if $e = 2^d - 1$ and $m = 0$ and $s = 0$, then $x = +$`Inf`
- if $e = 2^d - 1$ and $m = 0$ and $s = 1$, then $x = -$`Inf`
- if $0 < e < 2^d - 1$, the $x = (-1)^s \cdot (1.m)_2 \cdot 2^{e-b}$ (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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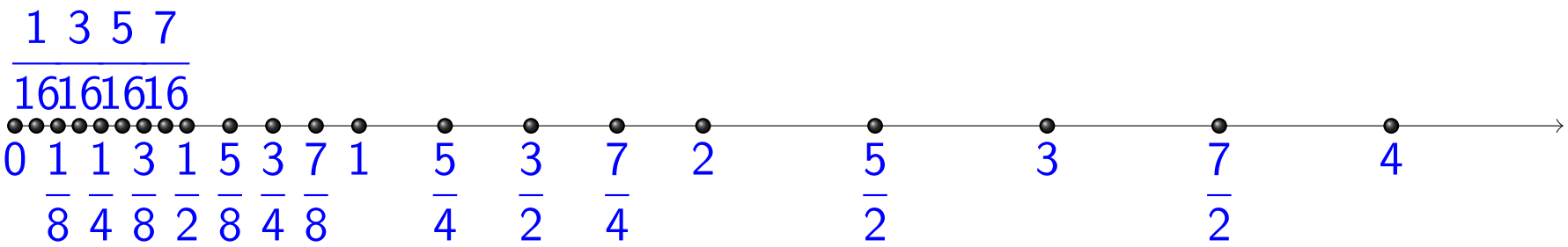
Example: take m of length 2 bits, e of length 3 bits, and $b = 3$.

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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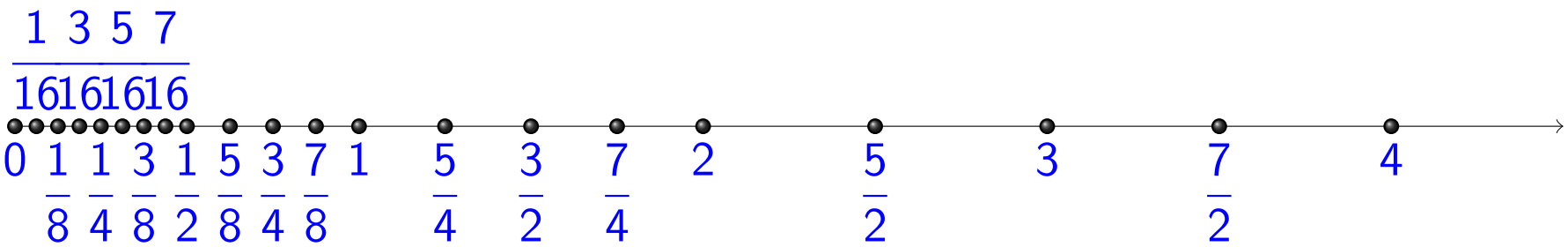

The set of all machine numbers with a given precision has little in common with real numbers. It resembles more to a finite subset of integers.

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} $\approx 2.2\cdot 10^{-308}$	$2^{-1022-52}=2^{-1074}$ $\approx 4.9\cdot 10^{324}$

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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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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* $\dfrac{|\alpha - a|}{|a|}$.

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

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

$$x = (1.b_1 b_2 b_3 b_4 \ldots)_2 \cdot 2^{\ell},$$

then

$$fl(x) = (1.b_1 b_2 \ldots b_{23}) \cdot 2^{\ell}.$$

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The absolute error is

$$|x - fl(x)| \leq 2^{-23+\ell}$$

and the relative error is

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

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This threshold of relative error is called the **unit roundoff error** and is denoted by **u**, i.e., 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

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

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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Let us calculate the relative error.

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Proposition

Let x and y be normalized machine numbers and $x > y > 0$.
*If $2^{-p} \leq 1 - \frac{y}{x} \leq 2^{-q}$ 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.

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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

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

vector of Euclidean length $\frac{1}{6}$ (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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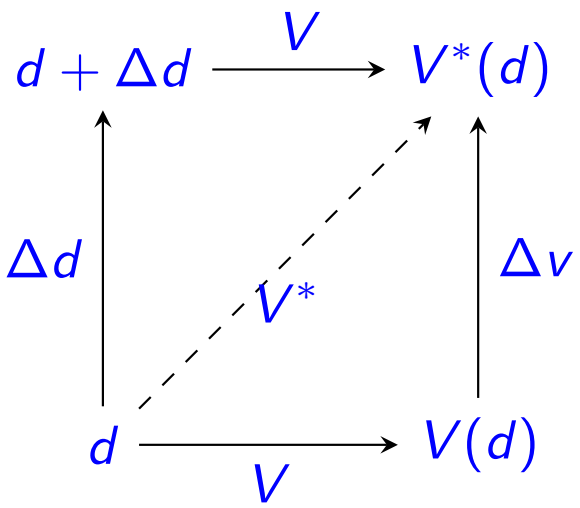
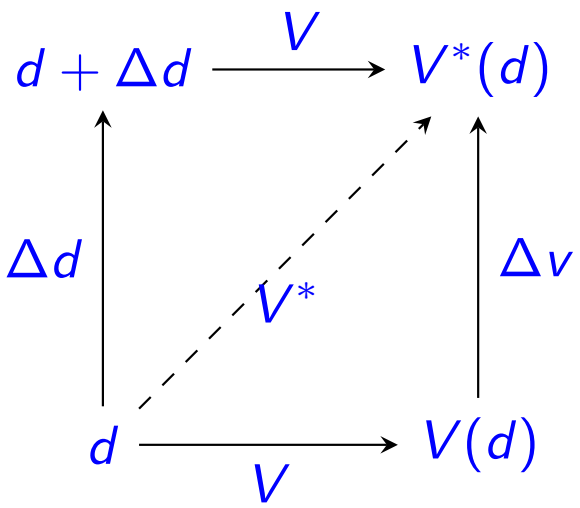


Forward and backward error

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**.



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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The **relative condition number** of a problem is

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

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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**.

Outline

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:

$$x_0, x_1, x_2, \ldots$$

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

Outline

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. $\|x\| = 0 \;\Rightarrow\; x = 0$,
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 $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$.

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Other commonly used norms include

- $\|x\|_\infty = \max\left\{ |x_i| : i \in \{1, \ldots, n\} \right\}$ 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,

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

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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 shall 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.

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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

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

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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 $\lim_{k\to+\infty} W^k = 0$.

Convergence vs. spectral radius

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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Theorem

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

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

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

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

Finite precision calculations

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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

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

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

Choices of Q

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

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

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 $Q = \frac{1}{\omega} D + L$.

Richardson method

Set $Q = I$.

The recurrence relation is given by

$$x_k = (I - A)x_{k-1} + b$$

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

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

SOR method

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

The recurrence relation is given by

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

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

Outline

Summary

We mentioned

- finite computer arithmetic and the most common problems when using it,
- different types of errors and their estimate,
- direct and iterative methods,
- basic iterative methods for systems of linear equations.