Lecture 0: Introduction and Terminology

A8B17CAS

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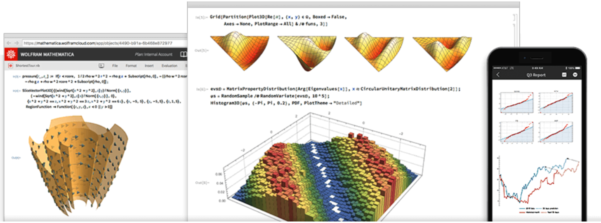
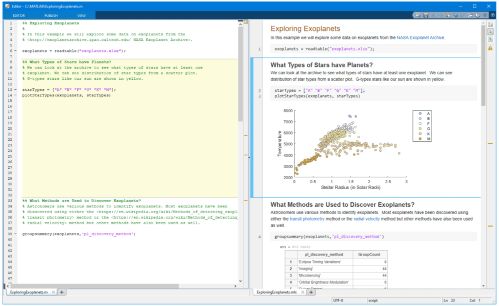
Outline

1. Programming and Numerical Computing Platforms
2. Why to Learn MATLAB & MATHEMATICA?
3. Basic Terms and Terminology
4. Example: A System of Linear Equations





Programming and Numerical Computing Platforms…

…help us with numerical and data analysis, i.e., to find an exact or approximate solution to numerical problems, analyze, modify, and present data, and develop algorithms and codes.

Common characteristics

- high-level programming languages (*4th generation*),
- excellent for "fast prototyping".

What Platforms Do We Have?

- They are many.
- From free & open-source to large & expensive systems.

▶ Software classification (wiki)

▶ List of numerical-analysis software (wiki)

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- We will focus on MATLAB and MATHEMATICA.

Why to learn MATLAB & MATHEMATICA?

- They are worldwide standards.
- They are used by thousands of universities worldwide.
- License used by a plethora of corporations in aviation, biotechnology, electronics, cybernetics, mechanical engineering, finance, ...

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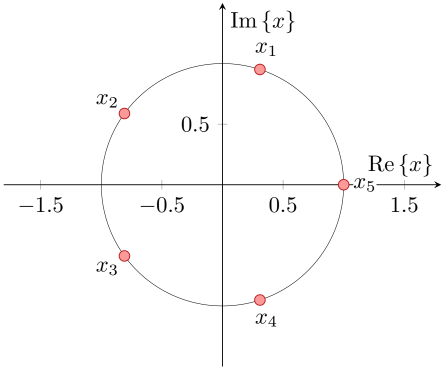
Where we can use them?

- Data processing and visualization during laboratory exercises.
- When elaborating diploma works.
- Seminar exercises (signals, algorithm development, . . .).
- Theory verification (mathematics and physics classes, electromagnetic field, electronic circuits, . . .).
- Studying aboard (Erasmus, Sokrates).
- In daily professional live.
- "everywhere" :)

Polynomial Roots (Problem Assignment)

Find polynomial roots x_n of

$$x^5 = 1.$$



Roots x_n of polynomial $x^5 = 1$ depicted in the complex plane.

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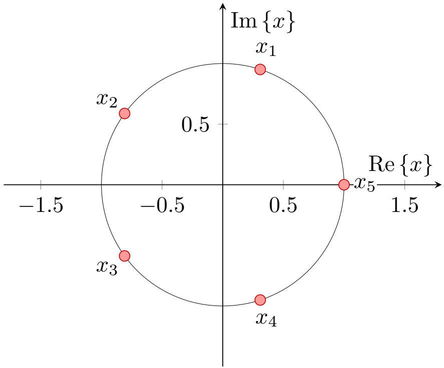
- We are lucky! All roots lie on the unitary circle in a complex plane, *i.e.*,

$$x_n = \exp\left\{\mathrm{j}\frac{2\pi n}{5}\right\} = (-1)^{(n-1)/5}, \quad i \in \{1, \ldots, 5\}.$$



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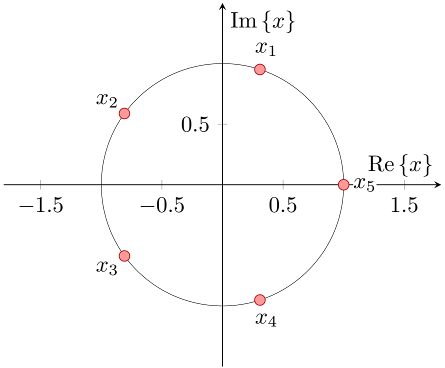

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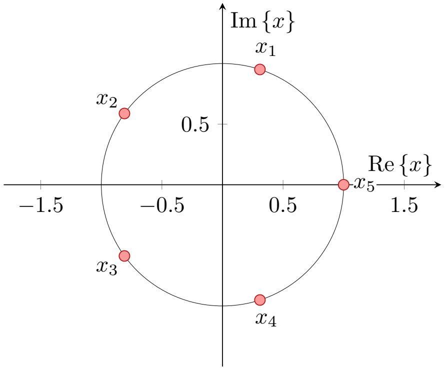
- Consequently, a numerical solution is required!



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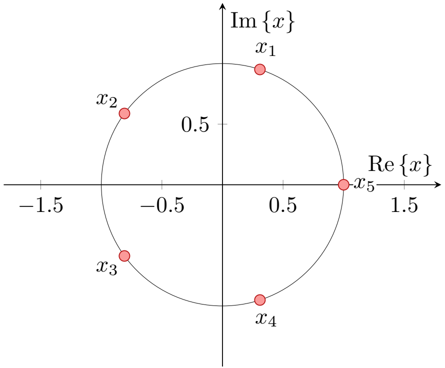
- Consequently, a numerical solution is required!
- Workflow: set up the problem, visualize if needed, solve, check, and present the data (results).



Roots x_n of polynomial $x^5 = 1$ depicted in the complex plane.

Polynomial Roots (Problem Solution: MATLAB)

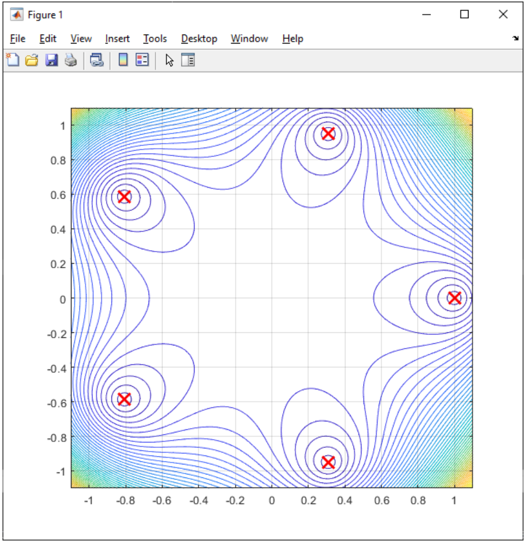
```
clear;

% Set up polynomial and find roots
p = [1 0 0 0 0 -1];
r = roots(p);

% Calculate data for visualisation
x = -1.1:1/100:1.1;
[Re, Im] = meshgrid(x, x.');
X = complex(Re, Im);
F = polyval(p, X);

% Plot the complex plane and the roots
contour(x, x, abs(F), 51);
hold on;
grid on;
plot(real(r), imag(r), 'rx', ...
   'MarkerSize', 15, 'LineWidth', 2);

% Analytical check
exp(1j*(0:(2*pi/5):(4*2*pi/5)))
```

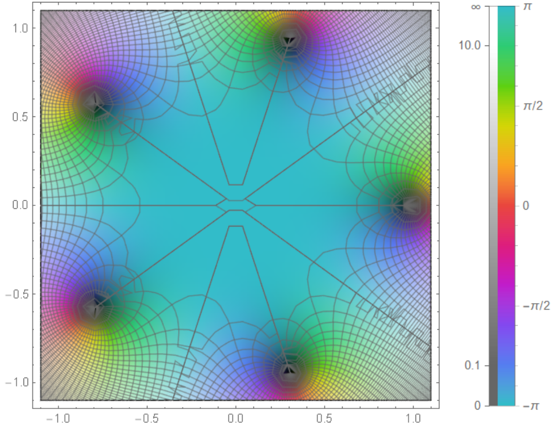


Polynomial Roots (Problem Solution: MATHEMATICA)

```
In[1]:= p = x^5 - 1;
        r = Roots[p == 0, x]
```

Out[2]= $x == 1 \,||\, x == (-1)^{2/5} \,||\, x == (-1)^{4/5} \,||\, x == -(-1)^{1/5} \,||\, x == -(-1)^{3/5}$

```
In[3]:= ComplexPlot[p, {x, -1.1 - 1.1 I, 1.1 + 1.1 I}, Mesh → 51,
         PlotLegends → Automatic, ColorFunction → "GlobalAbs"]
```



Analytical (Symbolic) $\times$ Numerical Evaluation

- "Analytical" solution to a problem is exact and obtained by methods of symbolic manipulation, derived using analysis.
  - When you do an "analytical solution" you answer to a whole set of problems, *e.g.*, $2a/a = 2 \quad \forall a$.
  - It provides generally valid results and often reveals the properties of the problem.

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- “Numerical” solution to a problem usually indicates an approximate solution obtained by methods of numerical analysis.
  - When you do a “numerical solution” you are generally only getting one answer, *e.g.*, $4/2 = 2$.
  - A particular solution that can be achieved for a large set of problems than the “analytical solution”.

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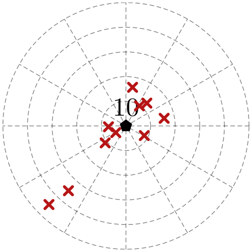
Example: The following doublets of MATHEMATICA commands lead to different results:
`2/4 = 1/2` vs. `N[2/4] = 0.5`, and `Pi` $= \pi$ vs. `N[Pi,5]` $= 3.1416$.

A Note on Difference Between Accuracy and Precision

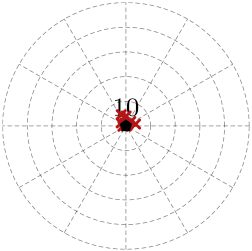
Be accurate: You are as close to the chosen goal/result as possible.

Be precise: You can repeat the evaluation/experiment as similarly as possible.

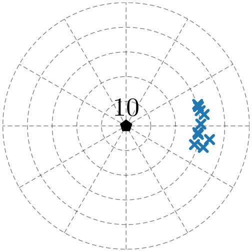
Example: Archery



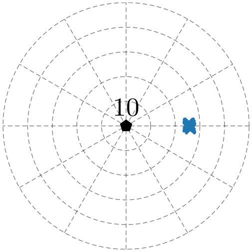
low accuracy



high accuracy



low precision



high precision

Compiled $\times$ Interpreted Language

Compiled language

- After compilation, the code is expressed in the instructions of the target machine.
- Compilation takes some time, but the final code is generally faster than the interpreted code (with a good compiler).

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- The code is executed line by line.
- Easier coding as compared to a compiled language.
- Allows execution of separate lines in arbitrary order (with easy on-fly modifications).
- All the debugging (and errors) occurs at run-time.

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There are advanced techniques sharing good properties of compiled and interpreted code.

- *e.g.*, JIT in MATLAB

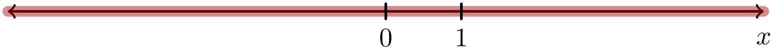
Type of Errors

In general, there are many types of errors:

- **Truncation** finite numerical precision
- **Discretization** continuous problem is solved point-wise, derivatives are replaced with differences, etc.
- **Modeling** intentional simplification of the model
- **Empirical constant** physical constants are used with a certain precision
- **Input** typos, intentionally incorrect input data, inaccurate measurement

Floating Point Numbers I.

Continuous axis or real numbers:



- Infinite resolution cannot be stored in computers based on finite arithmetic.

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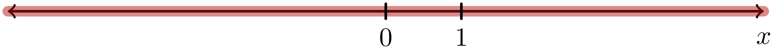

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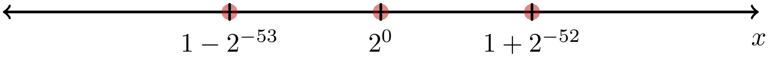
- IEEE 754 (Standard for Floating-Point Arithmetic)
- single precision (32 bits = 1 bit sign + 8 bits exponent + 23 bit mantissa)
- double precision (64 bits = 1 bit sign + 11 bits exponent + 52 bit mantissa)

Floating-point axis (in the vicinity of the number 1):



Floating Point Numbers II.

Decimal vs. sign-exponent-mantissa formats:

- $+2^0 = 1$

$=$ `0 01111111111 0000000000000000000000000000000000000000000000000000`

- $+2^0 \times (1 + 2^{-52}) \approx 1.0000000000000002$

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Be aware of finite-precision arithmetic:

```
>> cos(pi/2) = 6.123233995736766e-17
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See more at ▶ Floating Point Numbers (C. Moler) and ▶ Numerics and Error Analysis (Standford).

Nomenclature

Let us agree on some basic notation.

- Scalars a, vectors $\mathbf{a}$, matrices $\mathbf{A}$, arrays,
- equations $\times$ expressions,
- algebraic, logical, relational, bit-wise, set (and other) operators.

Distinguish between mathematical notation and syntax in a given software!

- For example, a vector $\mathbf{v} = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}^{\mathrm{T}}$ is created in MATLAB as `v = [1; 2; 3]`.

- Notice that all PDF materials are made in LaTeX (Beamer) in Overleaf.
- Graphics (whenever possible) is made in LaTeX package Ti*k*Z.

System of Linear Equations

Consider a generic system of linear equations of the form:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 &= b_1, \\ a_{21}x_1 + a_{22}x_2 &= b_2, \end{aligned} \tag{1}$$

which can be written in algebraic form as

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \tag{2}$$

where

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{bmatrix}, \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}.$$

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Considering the matrix $\mathbf{A}$ is non-singular, the solution is found as

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}. \tag{3}$$

System of Linear Equations – An Interpretation

Let us be more specific:

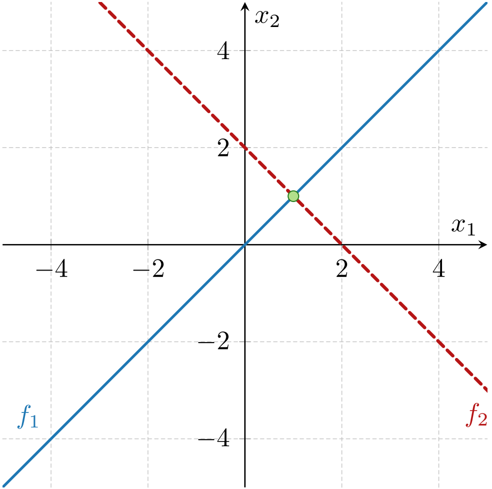
$$\begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Visual depiction by two lines, *i.e.*,

$$\begin{aligned} f_1 : \quad & x_1 = x_2, \\ f_2 : \quad & x_1 = 2 - x_2. \end{aligned}$$

MATLAB:

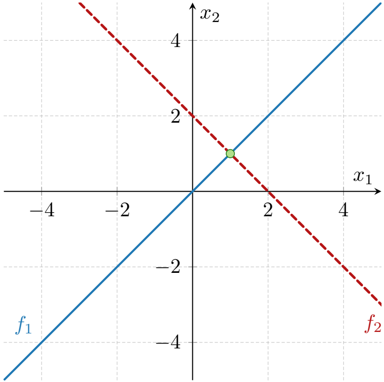
```
>> A = [1 -1; 1/2 1/2]
>> b = [0; 1]
>> x = A\b
```

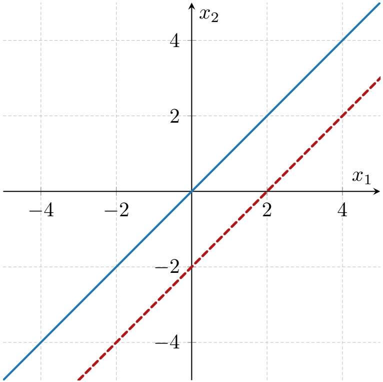


System of Linear Equations – Well- and Ill-Conditioned Problems

Looks like a piece of cake, however, be always careful…

$$\begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \Rightarrow \quad \mathbf{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \qquad \begin{bmatrix} 1 & -1 \\ 0.5 & -0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \Rightarrow \quad \mathbf{x} = \begin{bmatrix} ? \\ ? \end{bmatrix}.$$





System of Linear Equations – An Analysis of the Problem

- We will need: determinant, $\det(\mathbf{A})$, matrix inversion, $\mathbf{A}^{-1}$, dot product, $\mathbf{u} \cdot \mathbf{v}$, second norm of a vector, $\|\mathbf{u}\|$, condition number, $\operatorname{cond}(\mathbf{A})$.
- We have to investigate: how to approach the problem, the existence of a solution, accuracy of the results.
- We can try to find: a symbolic solution, extend the problem, and solve special cases.

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$$\det(\mathbf{A}) = a_{11}a_{22} - a_{12}a_{21}$$

```
>> det(A)
```

$$\mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})} \begin{bmatrix} +a_{22} & -a_{12} \\ -a_{21} & +a_{11} \end{bmatrix}$$

```
>> inv(A)
```

$$\mathbf{u} \cdot \mathbf{v} = \sum_i u_i v_i$$

```
>> dot(u,v)
```

$$\|\mathbf{u}\| = \sqrt{\mathbf{u} \cdot \mathbf{u}}$$

```
>> norm(u, 2)
```

$$\mathrm{cond}\,(\mathbf{A}) = \|\mathbf{A}\| \, \|\mathbf{A}^{-1}\|$$

```
>> cond(A)
```

System of Linear Equations – Generalization & Symbolic Solution

- Whenever possible, try to find a symbolic solution (good for verification and understanding of the problem's properties).

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Let us consider the following generalization $\mathbf{A} \longrightarrow \mathbf{A}(\kappa)$

$$\begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 - \kappa \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \kappa \in [0, 1],$$

covering all cases from well-defined ($\kappa = 0$) to ill-defined ($\kappa = 1$).

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$$\det(\mathbf{A}) = 1-\kappa, \qquad \mathbf{x} = \mathbf{A}^{-1}(\kappa)\,\mathbf{b} = \frac{1}{1-\kappa}\begin{bmatrix} 0.5-\kappa & 1 \\ -0.5 & 1 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{1-\kappa}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \Leftrightarrow \quad \kappa \neq 1.$$

System of Linear Equations – A Note on Angle Between f_1 and f_2

- To study the finite-precision performance of MATLAB depending on κ, let us express angle α between f_1 and $f_2(\kappa)$.
- Two possibilities shown:

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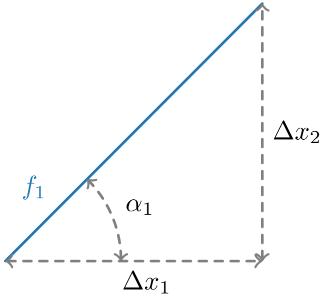
I. Trigonometry and a slope of the line:

$$f_1 : \quad x_2 = \frac{b_1 - a_{11}x_1}{a_{12}} \quad \text{and analogously for } f_2\left(\kappa\right)$$

$$f_1 : \quad \frac{\mathrm{d}x_2}{\mathrm{d}x_1} = -\frac{a_{11}}{a_{12}} = \tan\left(\alpha_1\right) \quad \text{and analogously for } f_2\left(\kappa\right)$$

$$|\alpha| = |\alpha_1 - \alpha_2| = \left|\arctan\left(-\frac{a_{11}}{a_{12}}\right) - \arctan\left(-\frac{a_{21}}{a_{22}}\right)\right|$$



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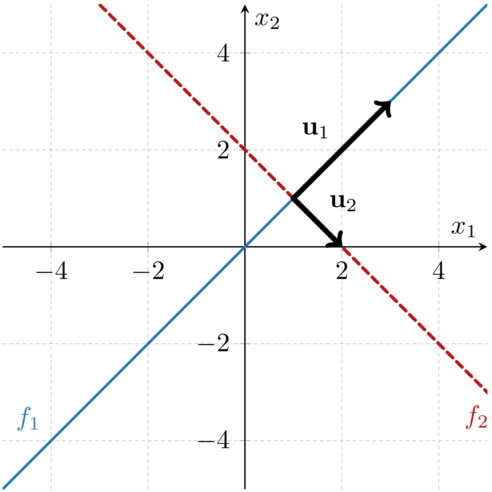
II. Property of the inner product:

$$\mathbf{u}_1 \cdot \mathbf{u}_2 = \|\mathbf{u}_1\| \, \|\mathbf{u}_2\| \cos(\alpha)$$

$$|\alpha| = \left| \arccos\left(\frac{\mathbf{u}_1 \cdot \mathbf{u}_2}{\|\mathbf{u}_1\| \, \|\mathbf{u}_2\|} \right) \right|$$

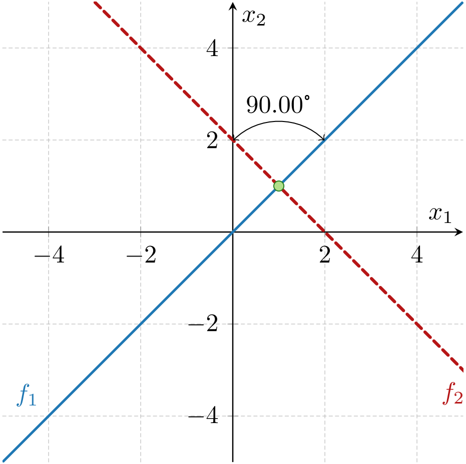
Normal vectors $\mathbf{u}_1$ and $\mathbf{u}_2$ along f_1 and f_2 are

$$\mathbf{u}_1 = c_1 \begin{bmatrix} a_{11} \\ -a_{12} \end{bmatrix}, \quad \mathbf{u}_2 = c_2 \begin{bmatrix} a_{21} \\ -a_{22} \end{bmatrix}.$$



System of Linear Equations – Parametric Study

- Since we know the analytical solution to the problem, we can compare MATLAB solution with it (depending on κ).
- As we should expect, the accuracy will be dependent on floating-point resolution.



MATLAB: $\kappa = 0.000000000000000$

$$x_1(\kappa) = 1.000000000000000$$
$$x_2(\kappa) = 1.000000000000000$$

$$|\det(\mathbf{A}(\kappa))| = 1.000000000000000$$
$$\mathrm{cond}(\mathbf{A}) = 2.000000000000000$$

MATLAB (double precision):

$$\kappa = 0.999999999000000$$

$$x_1(\kappa) = 1000000028.281932$$
$$x_2(\kappa) = 1000000028.281932$$

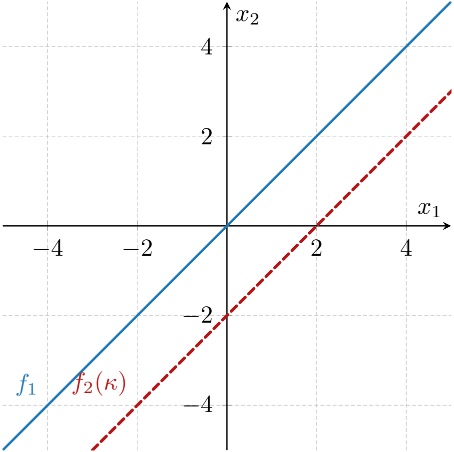
$$|\det(\mathbf{A}(\kappa))| = 0.000000001000000$$
$$\mathrm{cond}(\mathbf{A}) = 2500000205.439272$$

MATLAB (single precision):

$$\kappa = 0.999999999000000$$

$$x_1(\kappa) = \texttt{Inf}$$
$$x_2(\kappa) = \texttt{Inf}$$

$$|\det(\mathbf{A}(\kappa))| = 0.000000000000000$$
$$\mathrm{cond}(\mathbf{A}) = 163117008.0000000$$



MATLAB (double precision):

$$\kappa = 0.999999999000000$$

$$x_1(\kappa) = 1000000028.281932$$
$$x_2(\kappa) = 1000000028.281932$$

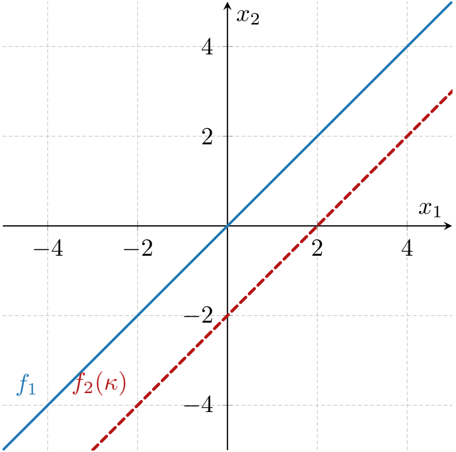
$$|\det(\mathbf{A}(\kappa))| = 0.000000001000000$$
$$\mathrm{cond}(\mathbf{A}) = 2500000205.439272$$

MATLAB (single precision):

$$\kappa = 0.999999999000000$$

$$x_1(\kappa) = \texttt{Inf}$$
$$x_2(\kappa) = \texttt{Inf}$$

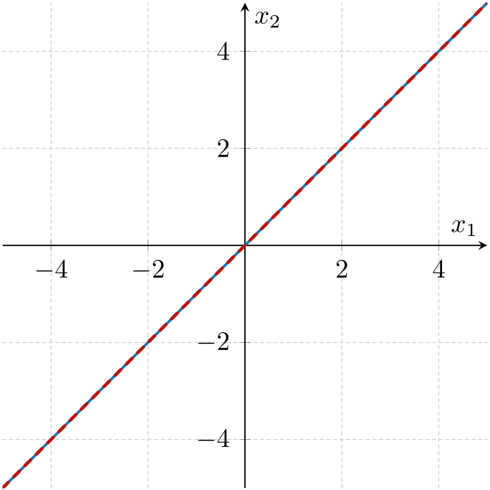
$$|\det(\mathbf{A}(\kappa))| = 0.000000000000000$$
$$\mathrm{cond}(\mathbf{A}) = 163117008.0000000$$



- Single precision gives finite results up to $\kappa \approx 1 - 10^{-7}$, since `eps(single(1))`$\approx 1.2 \cdot 10^{-7}$, *i.e.*, `abs(log2(eps(single(1)))) = 23`.
- Double precision gives finite results up to $\kappa \approx 1 - 10^{-16}$, since `eps(double(1))`$\approx 2.22 \cdot 10^{-16}$, *i.e.*, `abs(log2(eps(single(1)))) = 52`.

System of Linear Equations – On Special Cases

We are yet not finished!



System of Linear Equations – On Special Cases

- If the RHS of the problem

$$\begin{bmatrix} 1 & -1 \\ 0.5 & 0.5-\kappa \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

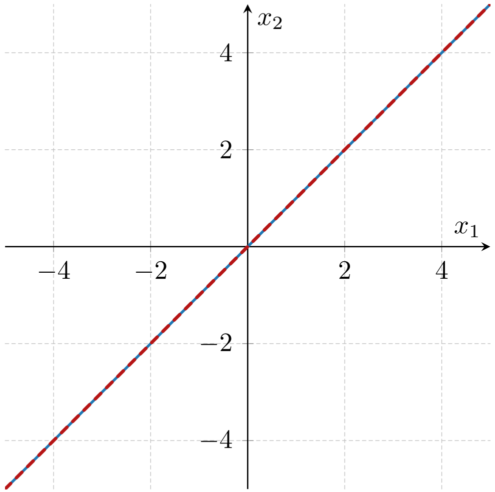
is changed to

$$\begin{bmatrix} 1 & -1 \\ 0.5 & 0.5-\kappa \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

we get for $\kappa \to 1$

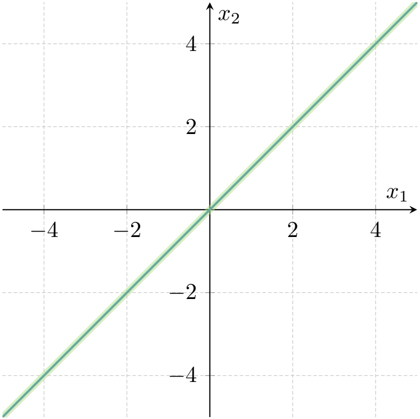
$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \frac{1}{1-\kappa} \begin{bmatrix} 0 \\ 0 \end{bmatrix} \to \infty \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \texttt{NaN} \\ \texttt{NaN} \end{bmatrix}.$$

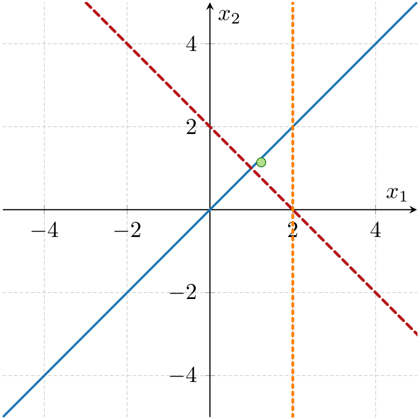
- Remember, sometimes, special cases lead to a very different solution!



System of Linear Equations – Under-/Over-determined Problems

$$\begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \end{bmatrix} \quad \text{to} \quad \begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 \\ 0.5 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$$





System of Linear Equations – Under-/Over-determined Problems

How to *a priori* recognize under-/over-determined system?

- Check rank of the matrix $\mathbf{A}$, MATLAB: `rank(A)`.
- Check the reduced echelon form of the augmented matrix, *i.e.*, `rref([A b])` in MATLAB. Is there any zero row?

Powerful techniques are still available (even inside lin. system solution via `mldivide` or `/`):

- Pseudo-inverse of a matrix, $\mathbf{A}^+$, MATLAB: `pinv(A)`.
- Least-square-sense solution, $\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|$.

In all cases:

- Be aware or check the condition number, MATLAB: `cond(A)`.

More about ▶ condition number of mathematical operations

System of Linear Equations – Final Remark (Linearity)

And . . . what if we make the following simple change?

$$\begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} x^2 \\ x^1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

System of Linear Equations – Final Remark (Linearity)

And ... what if we make the following simple change?

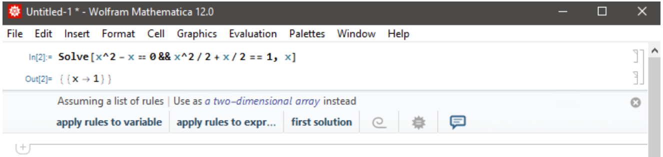
$$\begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} 1 & -1 \\ 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} x^2 \\ x^1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

No linearity anymore! Entering very different world (still, at least, the solution exist, $x = 1$).

MATLAB:

```
>> syms x
>> solve([x^2 - x == 0, ...
  1/2*x^2 + 1/2*x == 1], x)
```

MATHEMATICA:



Questions?

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