10.34: Numerical Methods Applied to Chemical Engineering

Lecture 1:
Organization,
Numerical Error,
Basics of Linear Algebra

Organization

- Purposes of the course:
    - Ensure that you are aware of the wide range of easily accessible numerical methods that will be useful in your thesis research, at practice school, and in your career.
    - Make you confident in your ability to look up and apply additional methods when you need them.
    - Help you become familiar with MATLAB, other convenient numerical software, and with simple programming/debugging techniques.
    - Give you an understanding of how common numerical algorithms work and why they sometimes produce unexpected results.

Organization

- Resources:
  - Course website – details on grading, homework policy, and homework submission guidelines.
  - Textbook – Beers, "Numerical Methods for Chemical Engineering". Notes will be placed on Course website. Additional text references are given in the syllabus.
  - MATLAB tutorials
  - Peers – you are encouraged to discuss the course material, programming, and the homework with your colleagues. Be aware of the homework policy outlined in the syllabus, however.
  - TAs and instructors – we are here to help you, and available for meetings, usually within 24 hours.

Organization

- When to stop:
  - The homework for the course should require 9 hours per week on average – perhaps a little more early on if you are not proficient with MATLAB.
  - Sometimes you may find a homework problem is consuming an inordinate amount of time even after you have asked for help.
  - If this happens, just turn in what you have completed with a note indicating that you know your solution is incomplete, details about what you think went wrong, and what you think a correct solution would look like.

Organization

- Linear algebra
- Solutions of nonlinear equations
- Optimization
- Initial value problems
- Differential-algebraic equations
- Boundary value problems
- Partial differential equations
- Probability theory
- Monte Carlo methods
- Stochastic chemical kinetics

Numerical Methods

- Motivation:
  - Most real engineering problems do not have an exact solution. Even if there is an exact solution. Can it be evaluated exactly?
  - Application of computational problem solving methodologies can lead to transformative (as opposed to incremental) engineering solutions.
- Algorithms to solve problems numerically should be:
  - clear
  - concise
  - able to solve the problem robustly
  - use realistic amount of resources
  - execute in a realistic amount of time

Numerical Error

- Virtually all computer problem solving is done approximately. It is essential to quantify the error in these calculations.

  - Example: representation of numbers

    $$\pi = 3.141592653589\ldots$$

    $$11001001000011111110110101$$

    significand (24 bits) exponent (8 bits)

    $$1 + \sum_{n=1}^{p-1} \mathrm{bit}_n \times 2^{-n} \Bigg) \times 2^e$$

  - Example: calculating the square root $\sqrt{s}$

    $$x^2 - s = 0$$

    Babylonian method (iterative solution):

    $$x_{n+1} = \frac{1}{2}\left(x_n + \frac{s}{x_n}\right)$$

Numerical Error

- Overflow/underflow – exceeding the largest/smallest representable number
  - Example: 1.3×10^{45} (nm)^3 =1.3×10^{9} (km)^3
  - Solution: rescaling
- Truncation:
  - Computers have a finite amount of memory/time to work with. Most algorithms work within these constraints to return answers which are accurate to within some tolerance.
  - Solution: the design of algorithms that quickly minimize truncation error
  - Example: Leibniz vs. Newton

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} = \frac{\pi}{4} \qquad \frac{1}{2}\sum_{n=0}^{\infty} \frac{2^n n!^2}{(2n+1)!} = \frac{\pi}{4}$$

Numerical Error

- Truncation (cont.):
  - Example: Leibniz vs. Newton

$$\sum_{n=0}^{N} \frac{(-1)^n}{2n+1} = \frac{\pi}{4} \qquad \frac{1}{2}\sum_{n=0}^{N} \frac{2^n n!^2}{(2n+1)!} = \frac{\pi}{4}$$

N	Leibniz	Newton
1	0.66667	0.66667
2	0.86667	0.73333
3	0.72381	0.76190
5	0.74401	0.78038
10	0.80808	0.78528

0.78540...

  - Absolute error:

$$\epsilon_{\text{abs.}} = \left|x_{\text{exact}} - x_{\text{approx.}}\right|$$

  - Relative error:

$$\epsilon_{\text{rel.}} = \frac{\left|x_{\text{exact}} - x_{\text{approx.}}\right|}{\left|x_{\text{exact}}\right|}$$

Numerical Error

- Truncation (cont.):
  - Example: $2 \times 10^{-4} + 1 \times 10^{-13}$ = ? with 8 digit accuracy
    - Estimate the absolute error in this calculation.
    - Estimate the relative error in this calculation.
- Quantifying and minimizing numerical error is a key aspect developing numerical algorithms.
- Even simple calculations introduce numerical errors.
  - Those errors can compound and magnify. We will see how shortly.

Linear Algebra

- Primarily concerned with the solutions of systems of linear equations
  - Is there a solution?
  - If there is a solution, is it a unique?
  - Is it possible to find the solution or family of solutions?
- Chemical engineering example: mass balances

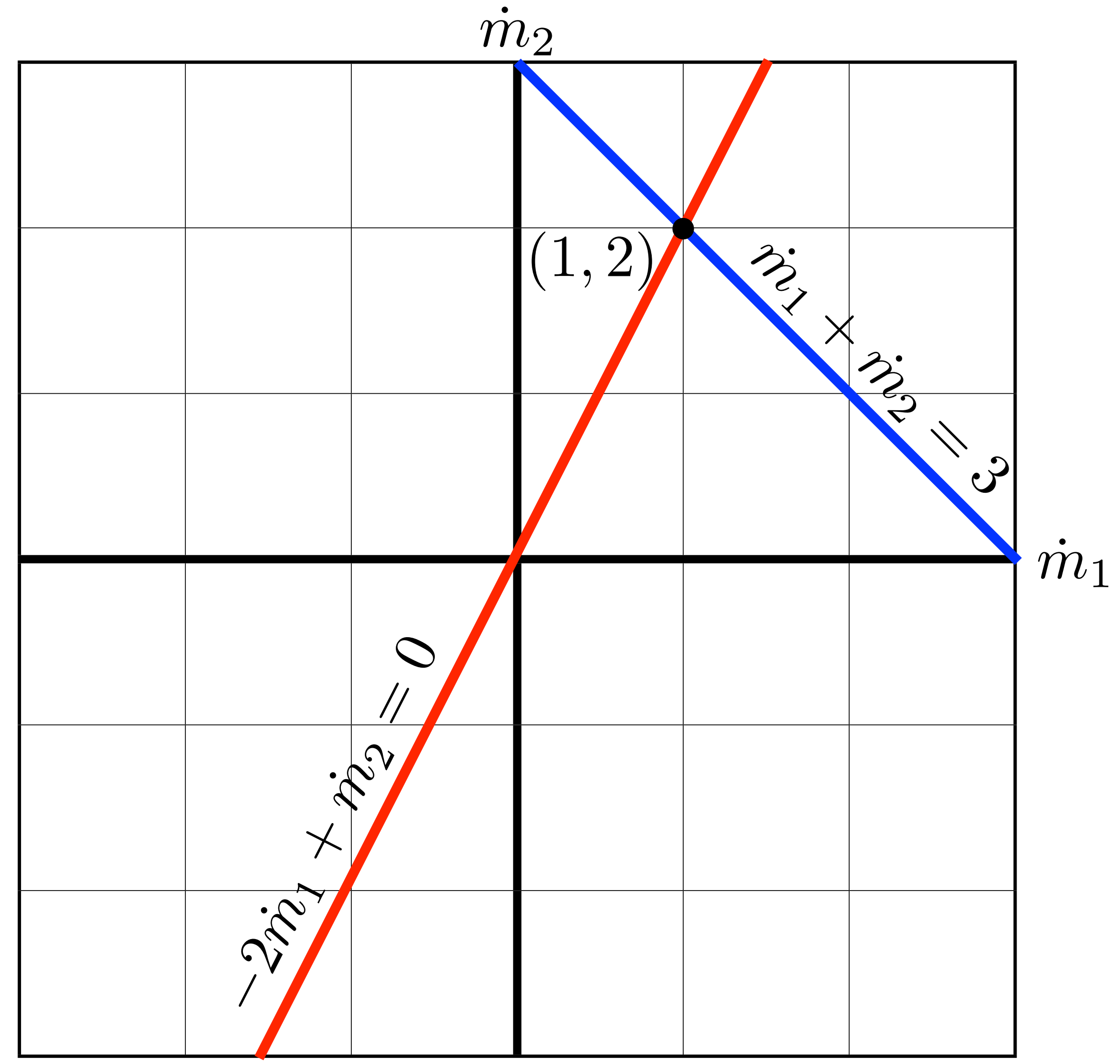
$$\dot{m}_1 + \dot{m}_2 = 3$$
$$\dot{m}_2 = 2\dot{m}_1$$

$$\begin{pmatrix} 1 & 1 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} \dot{m}_1 \\ \dot{m}_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 0 \end{pmatrix}$$

Linear Algebra

- Row-view:
  - Each row in the system of equations describes a line.
  - The solution represents the intersection of these lines.
  - For dimensions higher than 2, the solution is an intersection of other linear manifolds
  - How many solutions does the equation: ax=b, have?

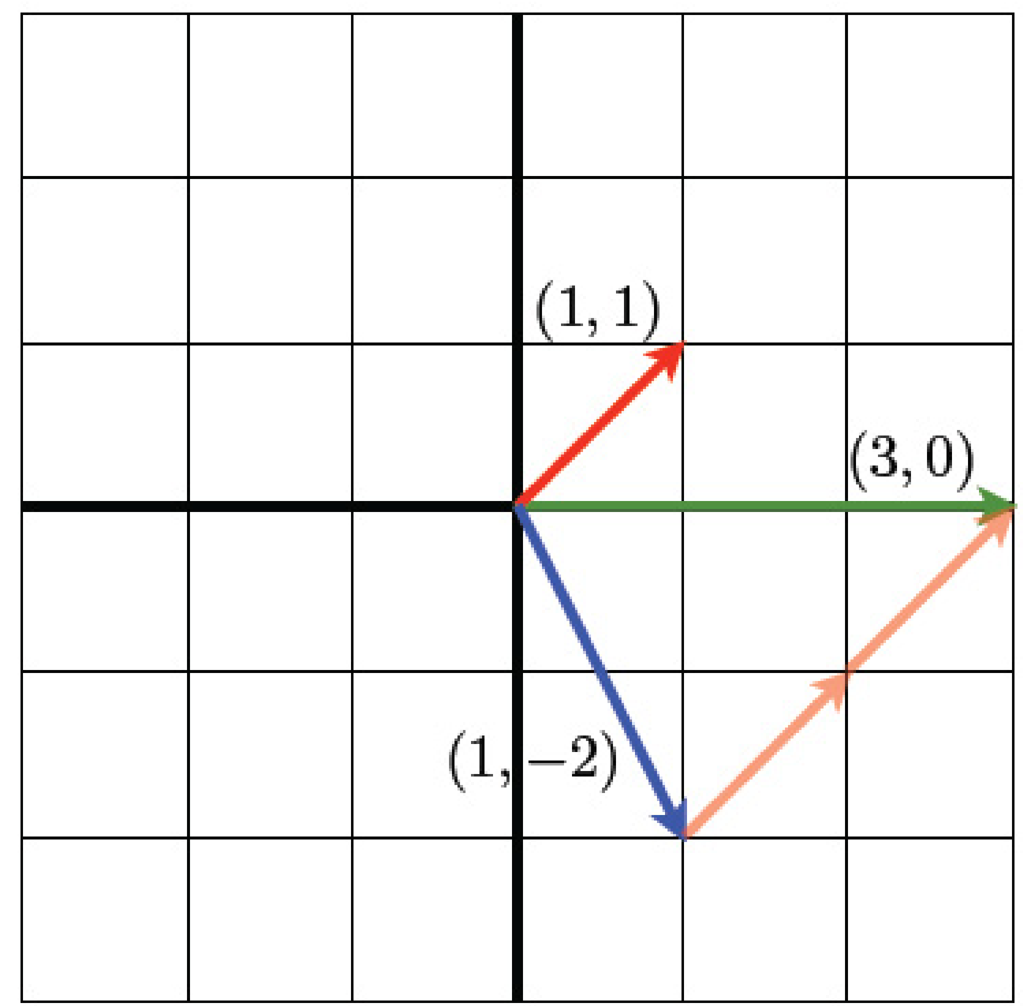
$$\begin{aligned} \dot{m}_1 &+ \dot{m}_2 &= 3 \\ -2\dot{m}_1 &+ \dot{m}_2 &= 0 \end{aligned}$$



Linear Algebra

- Column view:
  - Each column in the system of equations describes a vector.
  - The solution represents the correct weighting of these vectors.
  - While conceptually more difficult, the column view is easier to extend to arbitrarily high dimensions. You will see why later.

$$\dot{m}_1 \begin{pmatrix} 1 \\ -2 \end{pmatrix} + \dot{m}_2 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 3 \\ 0 \end{pmatrix}$$



Linear Algebra

Row-view:

$$\begin{pmatrix} -1 & 1 & 1 \\ 0 & -2 & 1 \end{pmatrix} \begin{pmatrix} \dot{m}_0 \\ \dot{m}_1 \\ \dot{m}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Column-view:

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} \dot{m}_2 \end{pmatrix} = \begin{pmatrix} 3-(1+\delta) \\ 2(1+\delta) \end{pmatrix}$$

Linear Algebra

Row-view:

$$\begin{pmatrix} -1 & 1 & 1 \\ 0 & -2 & 1 \end{pmatrix} \begin{pmatrix} \dot{m}_0 \\ \dot{m}_1 \\ \dot{m}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Column-view:

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} \dot{m}_2 \end{pmatrix} = \begin{pmatrix} 3 - (1 + \delta) \\ 2(1 + \delta) \end{pmatrix}$$

Solving Systems of Equations

$$ax = b \Rightarrow x = a^{-1}b$$

$$\mathbf{Ax} = \mathbf{b} \Rightarrow \mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

In MATLAB:

```
x = A \ b
```

Scalars, Vectors and Matrices

- Scalars:
  - Just single numbers!
  - Set of all real numbers, $\mathbb{R}$
  - Set of all complex numbers, $\mathbb{C}$
  - $i = \sqrt{-1}$
  - If $z \in \mathbb{C}$, then $z = a + ib$ with $a, b \in \mathbb{R}$
  - Complex conjugate: $\bar{z} = a - ib$
  - Magnitude: $|z| = \sqrt{z\bar{z}}$
  - $\mathbb{R} \subset \mathbb{C}$

Scalars, Vectors and Matrices

- Vectors:
  - Ordered sets of numbers: $(x_1, x_2, \ldots x_N)$
  - Set of all real vectors with dimension N, $\mathbb{R}^N$
  - Addition:

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} + \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_N + y_N \end{pmatrix}$$

  - Multiplication by scalar:

$$c(x_1 \ x_2 \ \ldots \ x_N) = (cx_1 \ cx_2 \ \ldots \ cx_N)$$

  - Transpose:

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} \qquad \mathbf{x}^T = (x_1 \ x_2 \ \ldots \ x_N)$$

Scalars, Vectors and Matrices

- Vectors:
  - Scalar product: $\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{N} x_i y_i$
  - Norm: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^{N} |x_i|^p \right)^{1/p}$
    - Properties:
      - Non-negative: $\|\mathbf{x}\|_p \geq 0$
      - If $\|\mathbf{x}\|_p = 0$, then $\mathbf{x} = 0$
      - $\|c\mathbf{x}\|_p = |c| \|\mathbf{x}\|_p$
      - $|\mathbf{x} \cdot \mathbf{y}| \leq \|\mathbf{x}\|_p \|\mathbf{y}\|_q$ with $p, q > 0, \; 1/p + 1/q = 1$
      - $\|\mathbf{x} + \mathbf{y}\|_p \leq \|\mathbf{x}\|_p + \|\mathbf{y}\|_p$

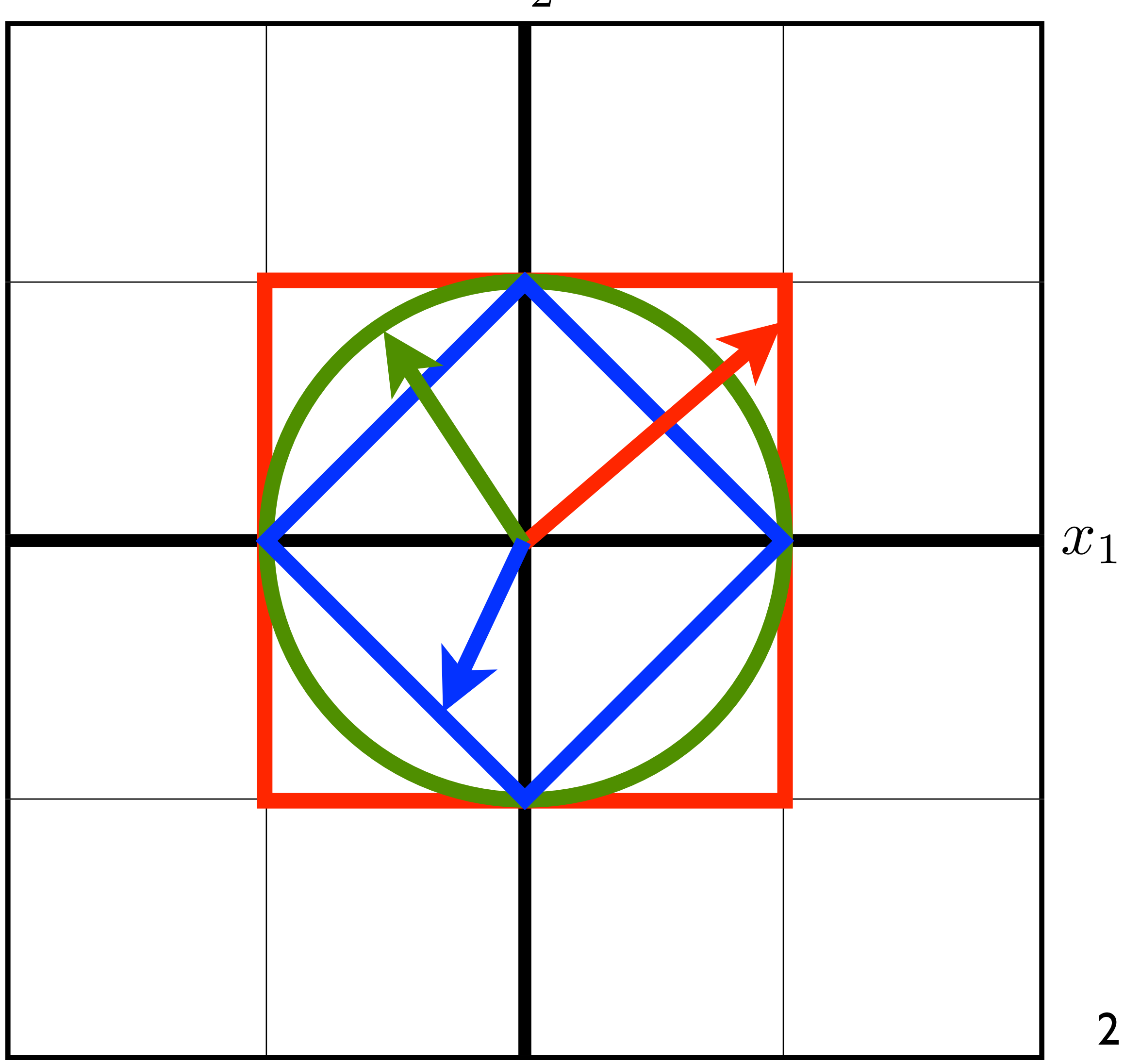
Scalars, Vectors and Matrices

- Vectors:
  - ∞-norm: $\|\mathbf{x}\|_\infty = \max_i |x_i|$
  - Examples of norms:

    $$\mathbf{x} = (\sqrt{2}/2, \sqrt{2}/2)$$

    - $\|\mathbf{x}\|_1 =$
    - $\|\mathbf{x}\|_2 =$
    - $\|\mathbf{x}\|_\infty =$
  - $\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_2 \leq \|\mathbf{x}\|_1$
  - Families of vectors with the same norm: 1-norm, 2-norm, ∞-norm

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^{N} |x_i|^p \right)^{1/p}$$



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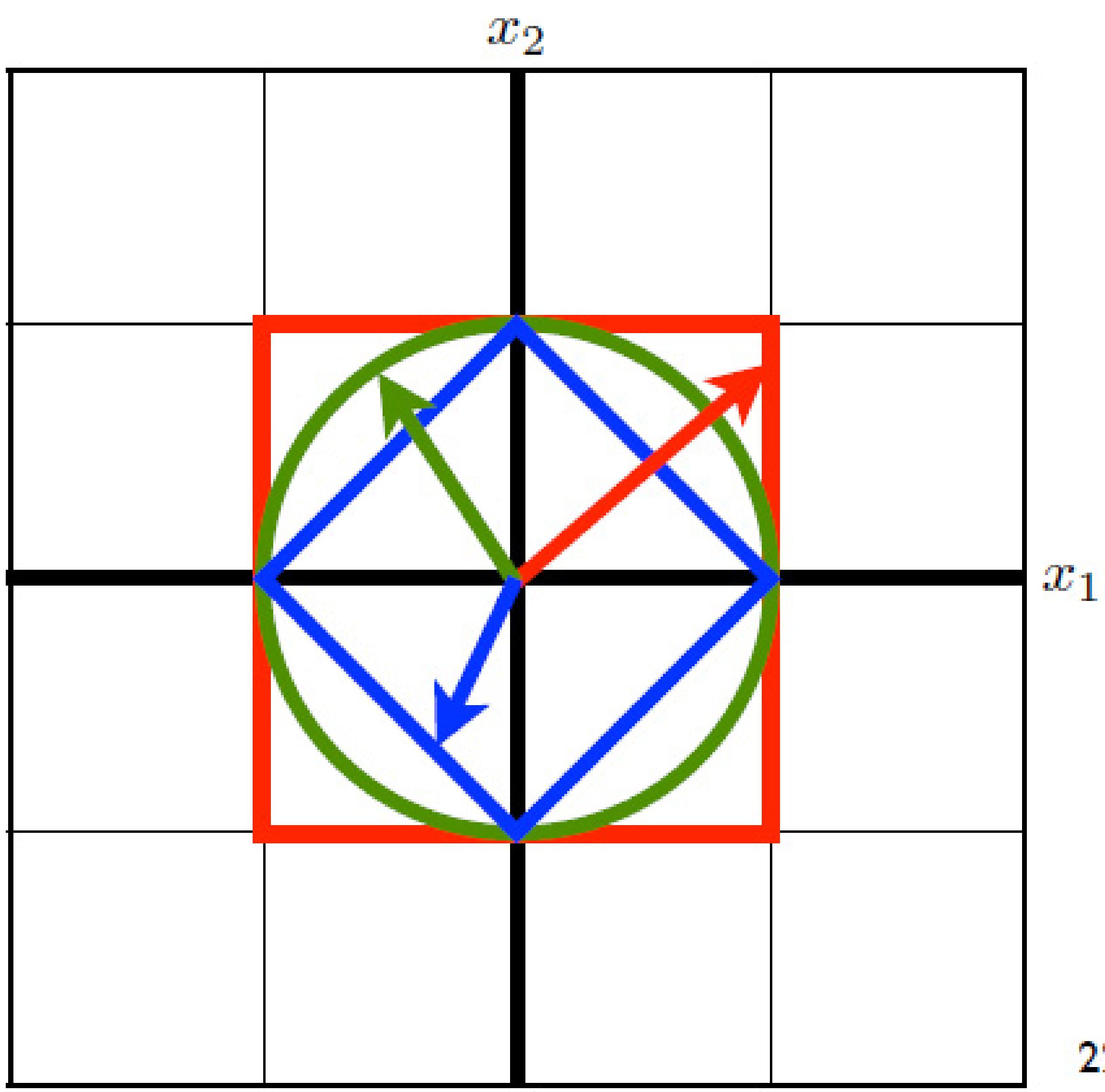
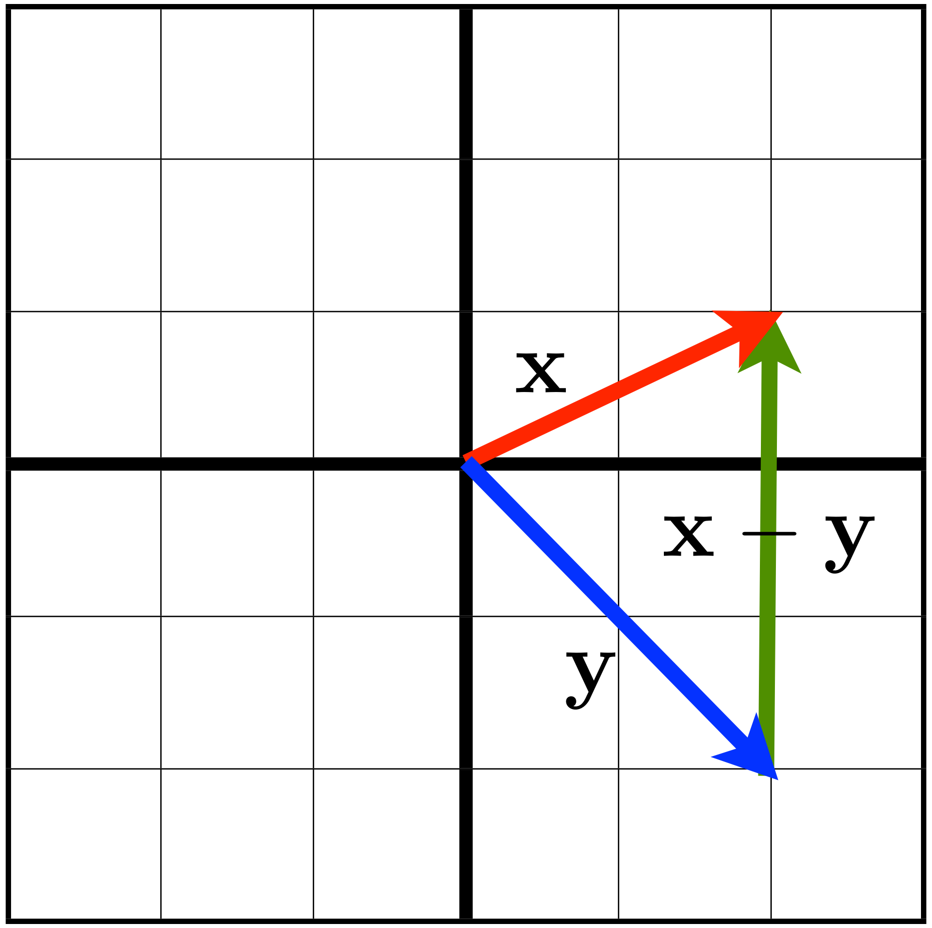


Scalars, Vectors and Matrices

- Vectors:
  - Comparing vectors with norm metrics:
    - $\|\mathbf{x} - \mathbf{y}\|_2 \geq 0$
    - If $\|\mathbf{x} - \mathbf{y}\|_2 = 0$, then $\mathbf{x} = \mathbf{y}$
    - $\|\mathbf{x} - \mathbf{y}\|_2 \leq \|\mathbf{x} - \mathbf{v}\|_2 + \|\mathbf{y} - \mathbf{v}\|_2$
  - Calculating norms in MATLAB:
    - `norm( x, p ), norm( x, Inf )`
  - How many operations to compute the norm?
  - How can I measure relative and absolute error for vectors?



Scalars, Vectors and Matrices

- Vectors:
  - Comparing vectors with norm metrics:
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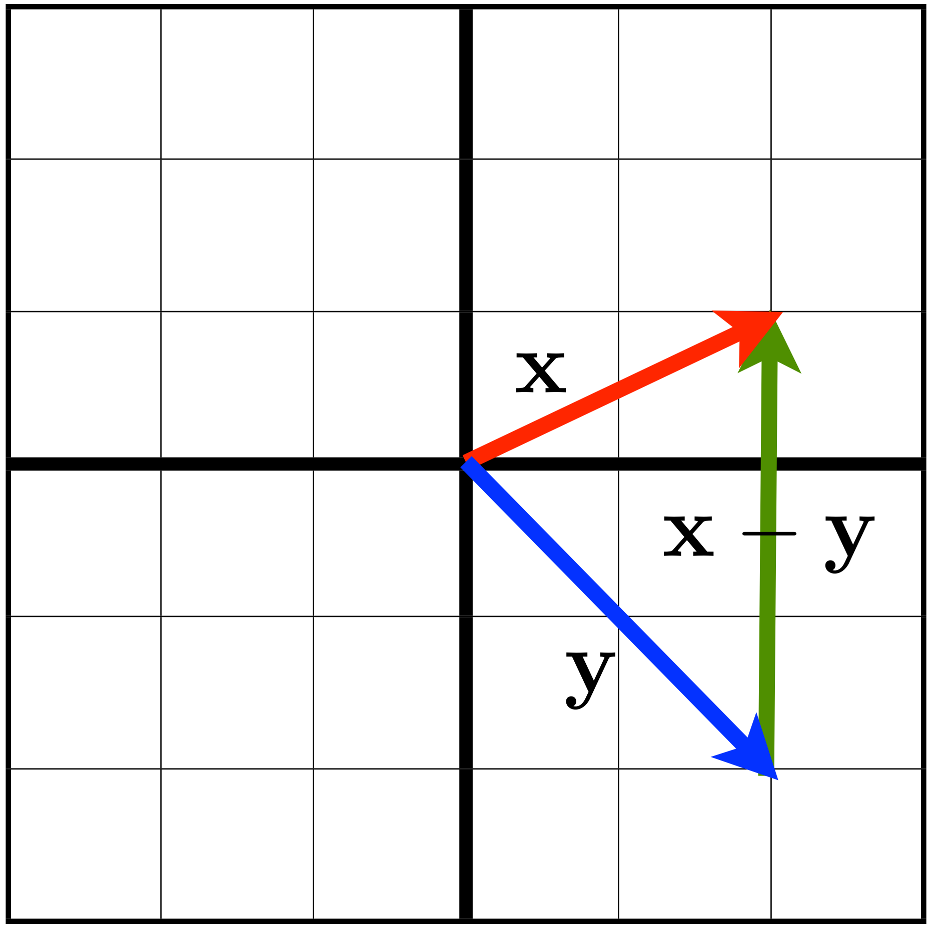
    - $\|\mathbf{x} - \mathbf{y}\|_2 \leq \|\mathbf{x} - \mathbf{v}\|_2 + \|\mathbf{y} - \mathbf{v}\|_2$
  - Calculating norms in MATLAB:
    - `norm( x, p ), norm( x, Inf )`
  - How many operations to compute the norm?
  - The relative and absolute error in a vector:



Scalars, Vectors and Matrices

- Vectors:
  - What mathematical object is the equivalent of an infinite dimensional vector?

Scalars, Vectors and Matrices

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Scalars, Vectors and Matrices

- Matrices:
  - Ordered sets of numbers:

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1M} \\ A_{21} & A_{22} & \dots & A_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \dots & A_{NM} \end{pmatrix}$$

  - Set of all real matrices with N rows and M columns, $\mathbb{R}^{N \times M}$
  - Addition: $\mathbf{C} = \mathbf{A} + \mathbf{B} \Rightarrow C_{ij} = A_{ij} + B_{ij}$
  - Multiplication by scalar: $\mathbf{C} = c\mathbf{A} \Rightarrow C_{ij} = cA_{ij}$
  - Transpose: $\mathbf{C} = \mathbf{A}^T \Rightarrow C_{ij} = A_{ji}$
  - Trace (square matrices):

$$\mathrm{Tr}\,\mathbf{A} = \sum_{i=1}^{N} A_{ii}$$

Scalars, Vectors and Matrices

- Matrices:
  - Matrix-vector product: $\mathbf{y} = \mathbf{A}\mathbf{x} \Rightarrow y_i = \sum_{j=1}^{M} A_{ij} x_j$
  - Matrix-matrix product: $\mathbf{C} = \mathbf{A}\mathbf{B} \Rightarrow C_{ij} = \sum_{k=1}^{M} A_{ik} B_{kj}$
    - Properties:
      - no commutation in general: $\mathbf{AB} \neq \mathbf{BA}$
      - association: $\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C}$
      - distribution: $\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{AB} + \mathbf{AC}$
      - transposition: $(\mathbf{AB})^T = \mathbf{B}^T \mathbf{A}^T$
      - inversion: $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$ if $\det(\mathbf{A}) \neq 0$

Scalars, Vectors and Matrices

- Matrices:
  - Matrix-matrix product:
    - Vectors are matrices too:
      - $\mathbf{x} \in \mathbb{R}^N \quad \mathbf{x} \in \mathbb{R}^{N \times 1}$
      - $\mathbf{y}^T \in \mathbb{R}^N \quad \mathbf{y}^T \in \mathbb{R}^{1 \times N}$
      - What is: $\mathbf{y}^T \mathbf{x}$?

$$\mathbf{C} = \mathbf{AB} \Rightarrow C_{ij} = \sum_{k=1}^{M} A_{ik} B_{kj}$$

Scalars, Vectors and Matrices

- Matrices:
  - Matrix-matrix product:
    - Vectors are matrices too:
      - $\mathbf{x} \in \mathbb{R}^N \quad \mathbf{x} \in \mathbb{R}^{N \times 1}$
      - $\mathbf{y}^T \in \mathbb{R}^N \quad \mathbf{y}^T \in \mathbb{R}^{1 \times N}$

      - What is: $\mathbf{y}^T \mathbf{x}$?

Scalars, Vectors and Matrices

- Matrices:
  - Dyadic product: $\mathbf{A} = \mathbf{x}\mathbf{y}^T = \mathbf{x} \otimes \mathbf{y} \Rightarrow A_{ij} = x_i y_j$
  - Determinant (square matrices only):

$$\det(\mathbf{A}) = \sum_{j=1}^{N} (-1)^{i+j} A_{ij} M_{ij}(\mathbf{A})$$

$$M_{ij}(\boldsymbol{A}) = \det \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1(j-1)} & A_{1(j+1)} & \dots & A_{1N} \\ A_{21} & A_{22} & \dots & A_{2(j-1)} & A_{2(j+1)} & \dots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ A_{(i-1)1} & A_{(j-1)2} & \dots & A_{(i-1)(j-1)} & A_{(i-1)(j+1)} & \dots & A_{(i-1)N} \\ A_{(i+1)1} & A_{(j+1)2} & \dots & A_{(i+1)(j-1)} & A_{(i+1)(j+1)} & \dots & A_{(i+1)N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \dots & A_{N(j-1)} & A_{N(j+1)} & \dots & A_{NN} \end{pmatrix}$$

- $\det(c) = c$

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