Root Finders and Solving Linear Systems

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(with basic contributions by Michael J. Dinneen
+ selected materials from slides by Michael T. Heath)

COMPSCI 369 Computational Science

1. Approximations with Taylor Series
2. Computing Roots of Equations
3. Review of Linear Algebra
4. Solving Systems of Linear Equations

Learning outcomes:

- Be familiar with basics of numerical analysis (scientific computing)
- Be familiar with methods for finding roots of equations
- Understand methods for solving systems of linear equations
- Understand that searching for roots of equations and solving linear systems appear in a wide range of scientific and engineering tasks

Notation:

$f'(x) \equiv \frac{d}{dx} f(x)$ – the 1st derivative of a function $f(x)$, e.g. $(x^2)' = 2x$

$f''(x) \equiv \frac{d^2}{dx^2} f(x)$ – the 2nd derivative of a function $f(x)$, e.g. $(x^2)'' = 2$

Taylor Series – Foundation of Numerical Methods

Representing a function $f : \mathbb{R} \to \mathbb{R}$ in neighbourhood of point $x = a$ (called a *centre*) by the values of the function and derivatives at a:

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \cdots + \frac{(x-a)^k}{k!}f^{(k)}(a) + \cdots$$

- For $a = 0$, the Taylor series is often called the McLaurin series

Taylor polynomial of degree n: $\widehat{f}_n(x;a) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k$

- The higher the degree, the more accurate the approximation of $f(x)$
- The polynomial $\widehat{f}_n(x;a)$ converges to $f(x)$ if $n \to \infty$
  - Often – only for certain values of x within the radius of convergence around the centre
  - Approximations in practical applications – for x close to a

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Example: Taylor Approximations of $f(x) = \exp(x) \equiv \mathrm{e}^x$

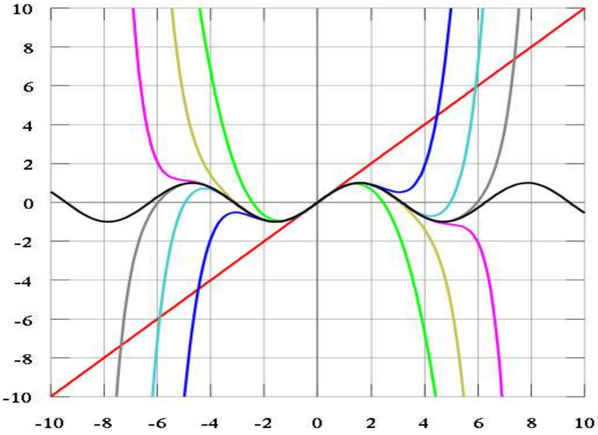
At $a = 0$, all the derivatives $\mathrm{e}^{(k)}(a) \equiv \frac{d^k}{dx^k}\mathrm{e}^x\Big|_{x=0} = \mathrm{e}^x|_{x=0} = 1$:

$$\widehat{e}_n(x;0) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{k=0}^{n} \frac{x^k}{k!}$$

- This power series converges to e^x everywhere: $\lim\limits_{n\to\infty} \widehat{e}_n(x) = e^x$

n	1	2	3	4	...	true e^x
$\widehat{e}_n(x=1;0)$	2.000000	2.500000	2.666667	2.708333	...	2.718282
Relative error; %	26	8.0	1.9	0.37		
$\widehat{e}_n(x=2;0)$	3.000000	5.000000	6.333333	7.000000	...	7.389056
Relative error; %	59	32	14	5.3		

Example: Taylor Approximations of $f(x) = \sin x$

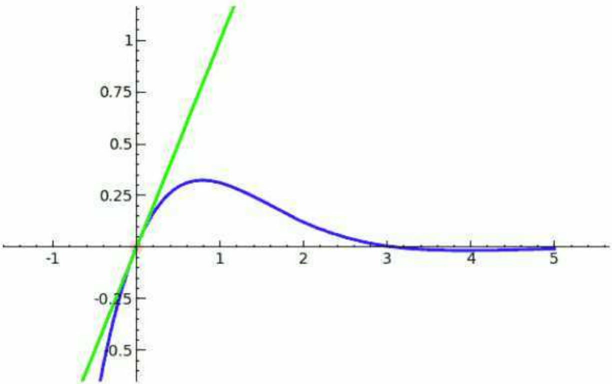


$f(x) = \sin x$ and Taylor approximations $\widehat{f}_n(x; 0)$ for $n = 1, 3, 5, 7, 9, 11,$ and 13

As the degree n rises, the Taylor polynomial approaches the correct function

Taylor Series Example (by H. Schilly)

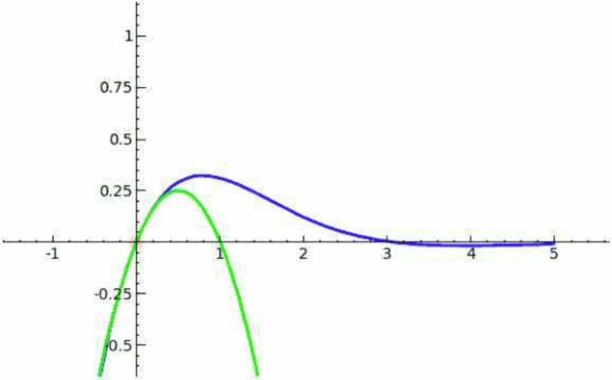
$$f(x) = e^{-x}\sin(x)$$
$$\hat{f}(x;0) = x + \mathcal{O}(x^2)$$



Taylor Series Example (by H. Schilly)

order 2

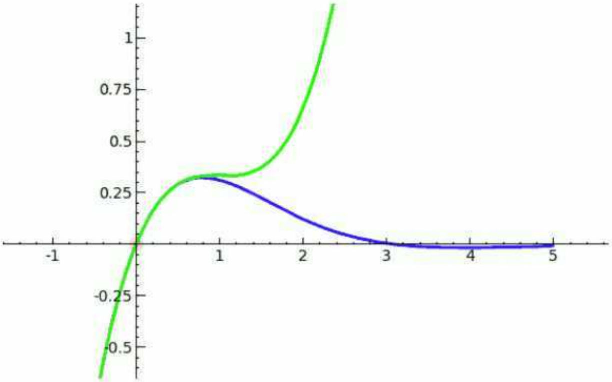
$$f(x) = e^{-x}\sin(x)$$
$$\hat{f}(x;0) = x - x^2 + \mathcal{O}(x^3)$$



Taylor Series Example (by H. Schilly)

order 3

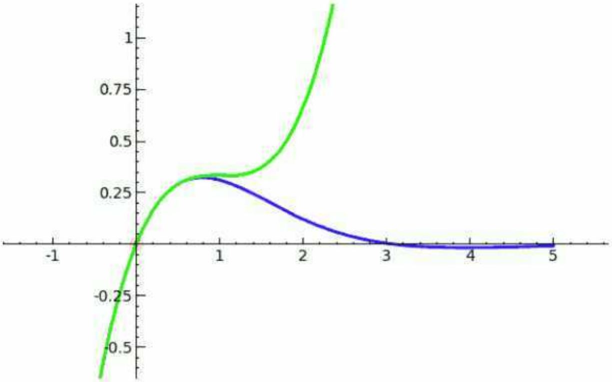
$$f(x) = e^{-x}\sin(x)$$
$$\hat{f}(x;0) = x - x^2 + \frac{x^3}{3} + \mathcal{O}(x^4)$$



Taylor Series Example (by H. Schilly)

order 4

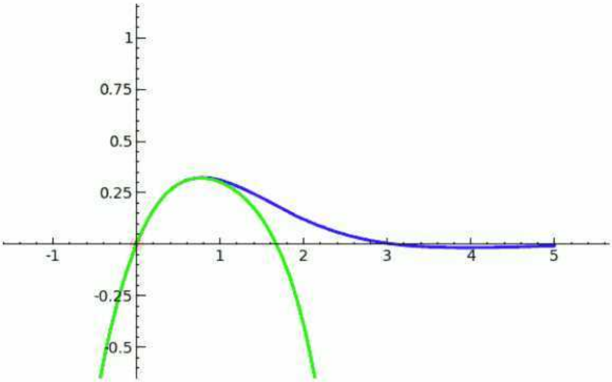
$$f(x) = e^{-x} \sin(x)$$
$$\hat{f}(x;0) = x - x^2 + \frac{x^3}{3} + \mathcal{O}(x^5)$$



Taylor Series Example (by H. Schilly)

order 5

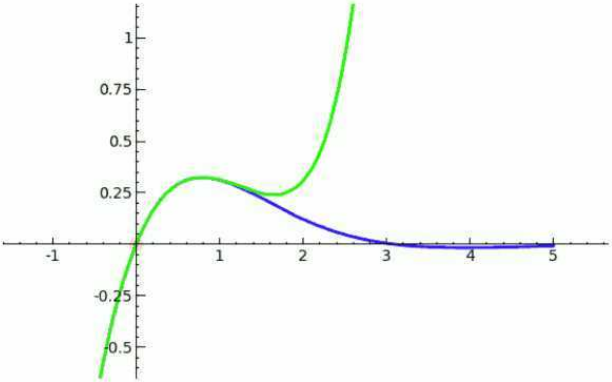
$$f(x) = e^{-x}\sin(x)$$
$$\hat{f}(x;0) = x - x^2 + \frac{x^3}{3} - \frac{x^5}{30} + \mathcal{O}(x^6)$$



Taylor Series Example (by H. Schilly)

order 6

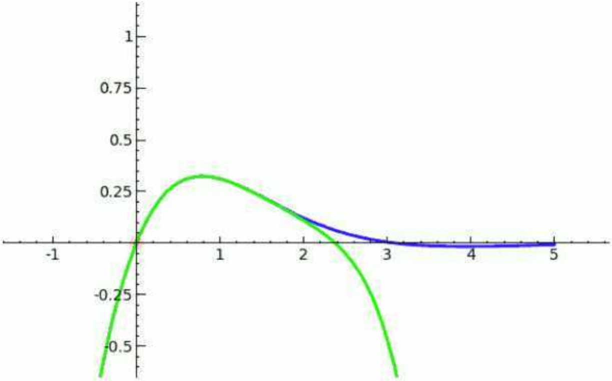
$$f(x) = e^{-x}\sin(x)$$
$$\hat{f}(x;0) = x - x^2 + \frac{x^3}{3} - \frac{x^5}{30} + \frac{x^6}{90} + \mathcal{O}(x^7)$$



Taylor Series Example (by H. Schilly)

order 7

$$f(x) = e^{-x} \sin(x)$$
$$\hat{f}(x;0) = x - x^2 + \frac{x^3}{3} - \frac{x^5}{30} + \frac{x^6}{90} - \frac{x^7}{630} + \mathcal{O}(x^8)$$



Taylor Series Example (by H. Schilly)

order 8

$$f(x) = e^{-x}\sin(x)$$
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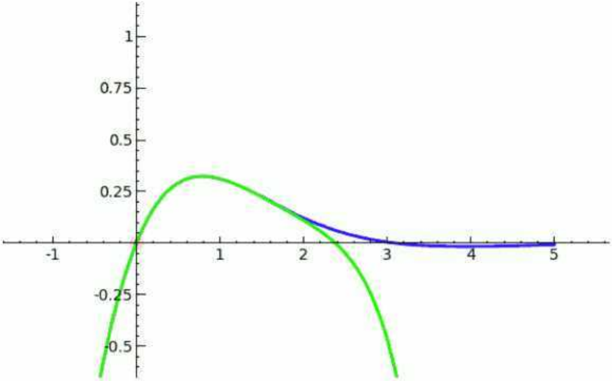
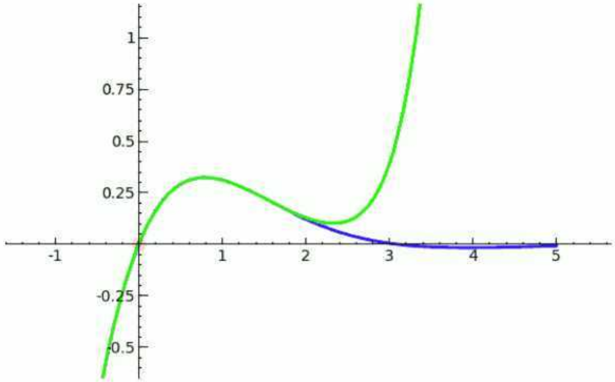


Taylor Series Example (by H. Schilly)

order 9

$$f(x) = e^{-x}\sin(x)$$
$$\hat{f}(x;0) = x - x^2 + \frac{x^3}{3} - \frac{x^5}{30} + \frac{x^6}{90} - \frac{x^7}{630} + \frac{x^9}{22680} + \mathcal{O}(x^{10})$$



Taylor Series Example (by H. Schilly)

order 10

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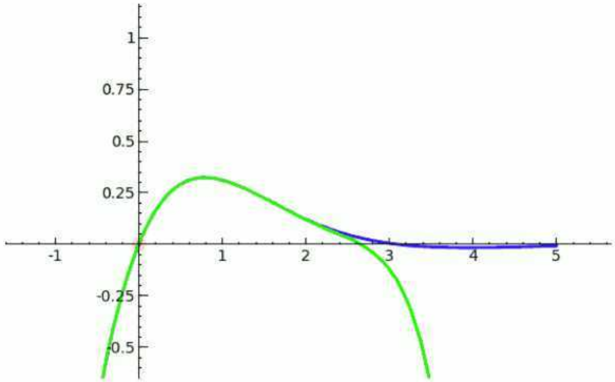

Taylor Series Example (by H. Schilly)

order 11

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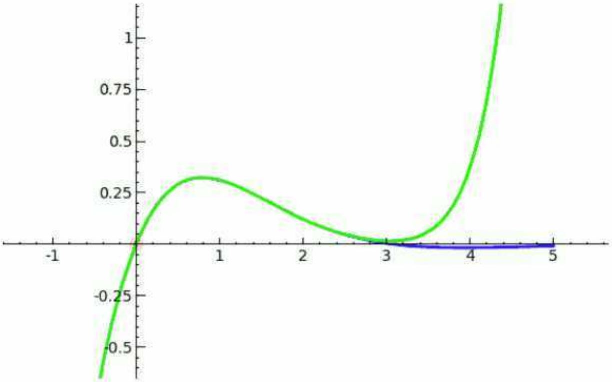

Taylor Series Example (by H. Schilly)

order 12

$$f(x) = e^{-x}\sin(x)$$
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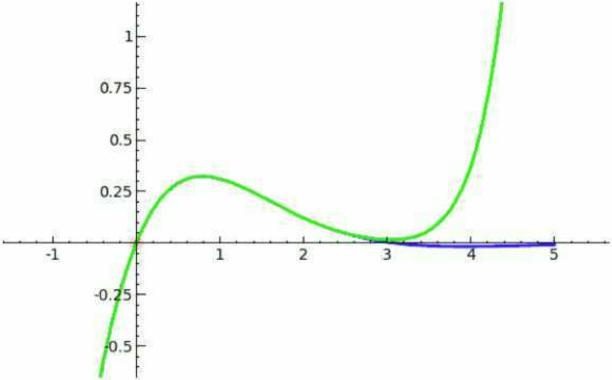

Convergence of a Sequence (an optional math info)

- Sequence $x_1, x_2, x_3, \ldots$ of real numbers converges to the number z if and only if for every real $\epsilon > 0$, there exists an integer N such that $|x_n - z| < \epsilon$ for every $n > N$
  - The limit z of the sequence $\{x_n\}$ (if exists) is considered as the exact solution of an iterative process producing x_n; $n = 1, 2. \ldots$
- Linear convergence to z, if there exists a number λ such that $\lim\limits_{n\to\infty} \frac{|x_{n+1}-x|}{|x_n-x|} = \lambda$; $0 < \lambda < 1$
  - The number λ is called the rate of convergence
  - Superlinear convergence if $\lambda = 0$; sublinear convergence if $\lambda = 1$
- Convergence with order α to z, if $\lim\limits_{n\to\infty} \frac{|x_{n+1}-x|}{|x_n-x|^\alpha} = \lambda > 0$ for $\alpha > 1$
  - Quadratic convergence – with order 2; cubic convergence – with order 3
  - More extended definitions of convergence exist, too

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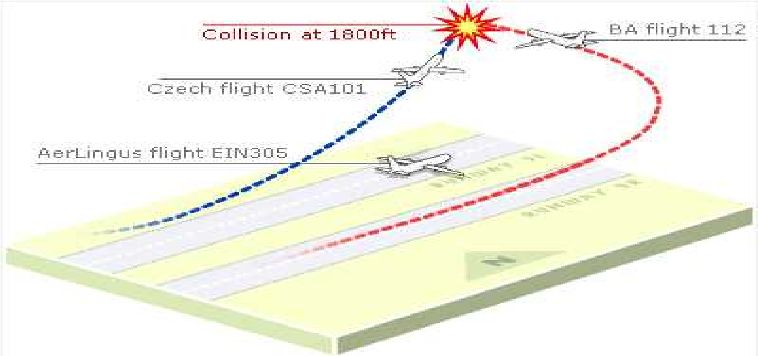
Numerical Root-Finding Algorithms

Root-finding algorithm – searching for an argument (root) x of a function $f : \mathbb{R} \to \mathbb{R}$, such that the function equals zero: $f(x) = 0$

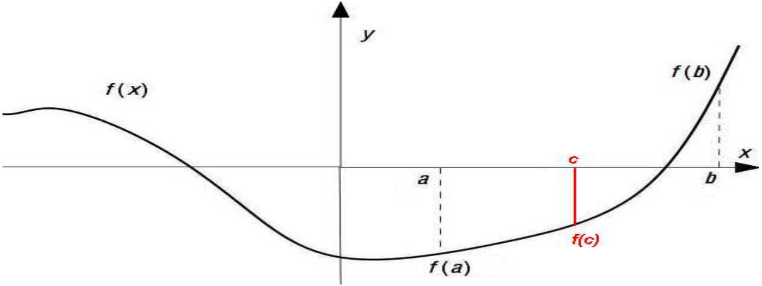
- Finding a root of $h(x) = f(x) - g(x)$ is the same as solving the equation $f(x) = g(x)$, i.e. finding x, such that $f(x) = g(x)$



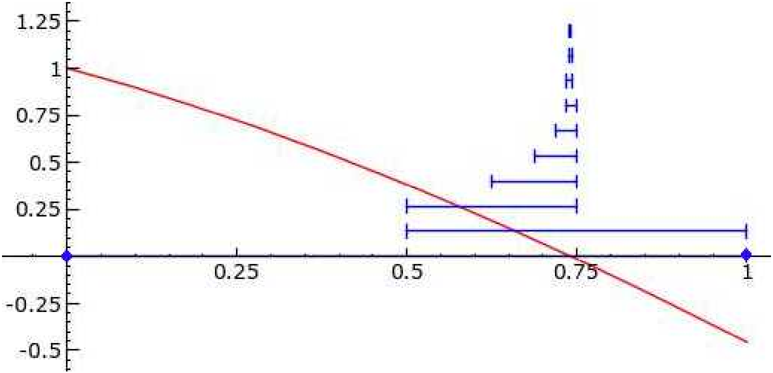
http://news.bbc.co.uk/nol/shared/spl/hi/programmes/the_day_britain_stopped/missed_approach/img/4_400.gif

Root-Finder: Bisection of a Continuous Function $f(x)$

- **Initialisation**: two guesses, a and b, such that $\operatorname{sign} f(a) \neq \operatorname{sign} f(b)$ (i.e. $f(a)$ and $f(b)$ have opposite signs)
- **Iterative search** until the absolute difference $|f(a) - f(b)| \approx 0$
  - Bisection: $c = a + \frac{b-a}{2} = \frac{a+b}{2}$
  - If $\operatorname{sign} f(a) = \operatorname{sign} f(c)$, then $a \leftarrow c$; otherwise $b \leftarrow c$
- Reliable, but slow convergence



Example: Bisection Method on $f(x) = \cos(x) - x$



Initial guesses: $a = 0; \quad f(0) = 1$

$b = 1; \quad f(1) = \cos(1) - 1 = -0.4597$

After 10 iterations:

root $c_9 = 0.7392578$; $f(0.7392578) = -0.0002890091\ldots$

Newton's Method: $f(x_n) + (x_{n+1} - x_n)\, f'(x_n) = 0$

- Based on the linear Taylor series expansion (first two terms):

$$f(x) \approx f(x_0) + (x - x_0) f'(x_0) = 0$$

- Next approximation (with quadratic convergence $\alpha = 2$):

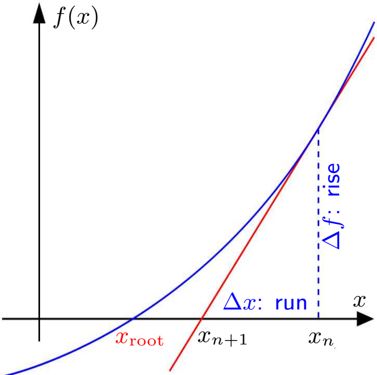
$$f'(x_n) = \frac{\text{rise}}{\text{run}} = \frac{\Delta f}{\Delta x} = \frac{f(x_n) - 0}{x_n - x_{n+1}}$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

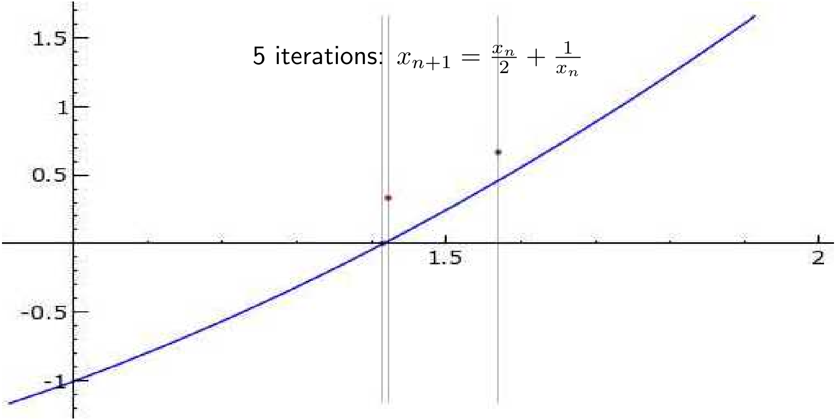
E.g. $f(x) = x^2 - 2$; $f'(x) = 2x$:

$$x_{n+1} = x_n - \frac{x_n^2 - 2}{2x_n}, \text{ i.e.}$$

$$x_{n+1} = \frac{x_n}{2} + \frac{1}{x_n}$$



Example: Newton's Method on $f(x) = x^2 - 2$



x_n	0.5	$\rightarrow$ 2.25	$\rightarrow$ 1.569444	$\rightarrow$ 1.421890	$\rightarrow$ 1.414234
$f(x_n)$	-1.75	3.065	0.463154	0.0217711	0.00005861552

True root value: $x_{\text{root}} = 1.41421356237\ldots$

A Few Other Common Root Finders (optional)

Secant method (http://en.wikipedia.org/wiki/Secant_method):

- Newton's method with a finite difference instead of the derivative
- Neither computation, nor existence of a derivative is required
- However, the convergence is slower (approximately, $\alpha = 1.6$)

False position method (http://en.wikipedia.org/wiki/False_position_method):

- Always retains one point on either side of the root
- Faster than the bisection and more robust than the secant method

Muller's method (http://en.wikipedia.org/wiki/Müller's_method):

- Quadratic (instead of linear) interpolations
- Faster convergence than with the secant method
- Roots may be complex (in addition to reals)

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Numerical Linear Algebra in Science and Engineering

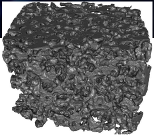
Numerical linear algebra is fundamental to all fields of science and engineering

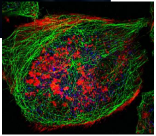
> *Most memory usage and computation time in optimization methods is spent on numerical linear algebra*
>
> — *Prof. S. Boyd, Standford University*

> *The field of numerical linear algebra is more beautiful, and more fundamental, than its rather dull name may suggest. . . . It is . . . really applied linear algebra . . . with the emphasis on practical algorithmic ideas rather than mathematical technicalities. . . . If any other mathematical topic is as fundamental to the mathematical sciences as calculus and differential equations, it is numerical linear algebra.*
>
> — *Lloyd N. Trefethen and David Bau:* Numerical Linear Algebra, *SIAM, 1997*

Numerical Linear Algebra in Science and Engineering

Economics, **chemistry**, **physics**, **industry**, **biotechnology**, **nanotechnology**: systems of discretised differential equations are solved using these tools





Air traffic control (collision avoidance); analysis of cellular materials; **bioinformatics**

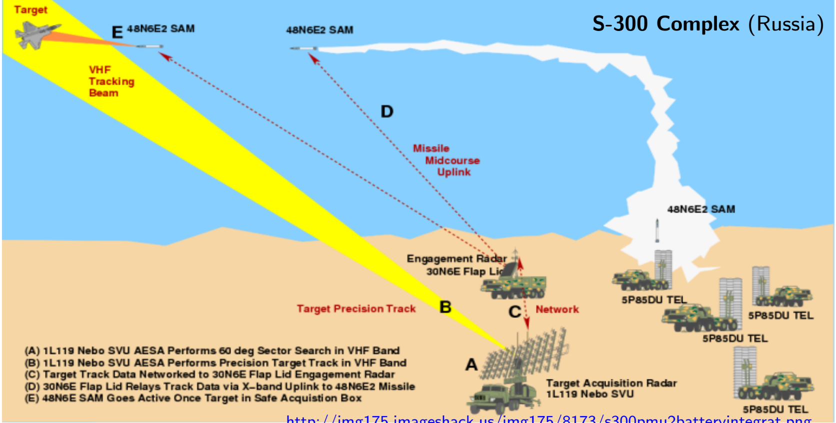
http://www.uni-due.de/imperia/md/images/css/niti_klein.jpg
http://www.mia.uni-saarland.de/Images/cell-small.jpg
http://www.p3air.com/wp-content/uploads/2011/02/plane_collision_1711510c.jpg
http://www.airlinetickets.org/wp-content/uploads/2010/11/near-collission.jpg

Numerical Linear Algebra in Science and Engineering

Google: the search engine computes with a monstrous sparse matrix of size $n = 4$ billion (see http://introcs.cs.princeton.edu/95linear/)

Military applications: missile guidance, autonomous navigation, ...

S-300 Complex (Russia)



http://img175.imageshack.us/img175/8173/s300pmu2batteryintegrat.png

Review of Linear Algebra (optional)

Inner (dot) product of vectors $\mathbf{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$ is the scalar $c = \mathbf{a} \bullet \mathbf{b} \equiv \mathbf{a}^\mathsf{T}\mathbf{b} = \sum_{i=1}^{n} a_i b_i$

$$\underbrace{\begin{bmatrix} 1 \\ -3 \\ 7 \end{bmatrix}}_{\mathbf{a}} \bullet \underbrace{\begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}}_{\mathbf{b}} = \underbrace{[1 \quad -3 \quad 7]}_{\mathbf{a}^\mathsf{T}} \underbrace{\begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}}_{\mathbf{b}}$$

$$= \underbrace{1 \cdot 2 - 3 \cdot 1 + 7 \cdot 1 = 2 - 3 + 7}_{a_1 b_1 + a_2 b_2 + a_3 b_3} = 6$$

Dot product is also called *multiplication* of vectors

Review of Linear Algebra, continued

Product of an $m \times n$ matrix $\mathbf{A} = \begin{bmatrix} A_{11} & \dots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \dots & A_{mn} \end{bmatrix}$ and an $n \times 1$ (n-dimensional) vector $\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$ is the m-dimensional vector $\mathbf{y} = \mathbf{Ax}$ with the elements $y_i = \sum_{j=1}^{m} A_{ij} x_j$

$$\underbrace{\begin{bmatrix} 2 & -1 & 2 \\ 1 & 3 & 3 \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} \overbrace{2 \cdot 2 - 1 \cdot 1 + 2 \cdot 1}^{A_{11}x_1 + A_{12}x_2 + A_{13}x_3} \\ \underbrace{1 \cdot 2 + 3 \cdot 1 + 3 \cdot 1}_{A_{21}x_1 + A_{22}x_2 + A_{23}x_3} \end{bmatrix} = \begin{bmatrix} 5 \\ 8 \end{bmatrix}}_{\mathbf{y}}$$

Review of Linear Algebra, continued

Product of a $k \times m$ matrix $\mathbf{A}$ and an $m \times n$ matrix $\mathbf{B}$ is the $k \times n$ matrix $\mathbf{C} = \mathbf{AB}$ with the elements $C_{ij} = \sum_{\alpha=1}^{m} A_{i,\alpha} B_{\alpha,j}$

$$\underbrace{\begin{bmatrix} 2 & -1 & 2 \\ 1 & 3 & 3 \end{bmatrix}}_{\mathbf{A}=\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{bmatrix}} \underbrace{\begin{bmatrix} 1 & 4 \\ 3 & 2 \\ -4 & 1 \end{bmatrix}}_{\mathbf{B}=\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \\ B_{31} & B_{32} \end{bmatrix}} = \underbrace{\begin{bmatrix} \overbrace{2\cdot 1 - 1\cdot 3 - 2\cdot 4}^{A_{11}B_{11}+A_{12}B_{21}+A_{13}B_{31}} & \overbrace{2\cdot 4 - 1\cdot 2 + 2\cdot 1}^{A_{11}B_{12}+A_{12}B_{22}+A_{13}B_{32}} \\ \underbrace{1\cdot 1 + 3\cdot 3 - 3\cdot 4}_{A_{21}B_{11}+A_{22}B_{21}+A_{23}B_{31}} & \underbrace{1\cdot 4 + 3\cdot 2 + 3\cdot 1}_{A_{21}B_{12}+A_{22}B_{22}+A_{23}B_{32}} \end{bmatrix}}_{\mathbf{C}=\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}}$$

Review of Linear Algebra, continued

Determinant of an $n \times n$ matrix A:

$$\det(A) \equiv |\mathbf{A}| = \sum_{\boldsymbol{\sigma} \in \mathbb{S}_n} (-1)^{\mathrm{inv}(\boldsymbol{\sigma})} \prod_{i=1}^{n} A_{i\sigma_i}$$

- $\mathbb{S}_n$ – the set of all the $n!$ permutations of the numbers $\{1, 2, ..., n\}$
- The sum over all the permutations $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_n) \in \mathbb{S}_n$
- $\mathrm{inv}(\boldsymbol{\sigma})$ – the number of *inversions* in $\boldsymbol{\sigma}$ (recall COMPSCI 220)

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = \begin{cases} & A_{11}A_{22}A_{33} & - & A_{11}A_{23}A_{32} \\ + & A_{12}A_{23}A_{31} & - & A_{12}A_{21}A_{33} \\ + & A_{13}A_{21}A_{32} & - & A_{13}A_{22}A_{31} \end{cases}$$

$\mathrm{inv}(1,2,3) = 0;\ \mathrm{inv}(1,3,2) = \mathrm{inv}(2,1,3) = 1;$
$\mathrm{inv}(2,3,1) = \mathrm{inv}(3,1,2) = 2;\ \mathrm{inv}(3,2,1) = 3$

Review of Linear Algebra, continued

The determinant can be used to find eigenvalues of a square matrix $\mathbf{A}$

- The eigenvalues are the roots of the *characteristic polynomial* $p(\lambda) = \det(\mathbf{A} - \lambda\mathbf{I})$ where $\mathbf{I}$ is the identity matrix of the same dimension as $\mathbf{A}$
  - Example for a 2×2 matrix $\mathbf{A}$:

$$\det(\mathbf{A} - \lambda\mathbf{I}) \equiv \begin{vmatrix} A_{11} - \lambda & A_{12} \\ A_{21} & A_{22} - \lambda \end{vmatrix}$$

$$\Rightarrow \quad p(\lambda) = \lambda^2 - (A_{11} + A_{22})\,\lambda + A_{11}A_{22} - A_{12}A_{21} = 0$$

- An eigenvector $\mathbf{A}\mathbf{e} = \lambda\mathbf{e}$
  - Transformation of the eigenvector $\mathbf{e}$ by multiplying (on the left) the matrix $\mathbf{A}$ simply scales this vector, $\lambda\mathbf{e}$, by the eigenvalue λ
  - Note: $\mathbf{A}^k\mathbf{e} = \lambda^k\mathbf{e}$

Review of Linear Algebra, continued

- An $m \times m$ matrix $\mathbf{A}$ has m orthogonal eigen-vectors $\mathbf{e}_1, \ldots, \mathbf{e}_m$:
  - → Mutual orthogonality: $\mathbf{e}_i \bullet \mathbf{e}_j = 0$ if $i \neq j$; $i, j \in \{1, 2, \ldots, m\}$
  - → Normalised eigenvectors: $\mathbf{e}_i \bullet \mathbf{e}_i = 1$
- **Eigen-vector representation** of the matrix: $\mathbf{A} = \sum_{i=1}^{m} \lambda_i \underbrace{\mathbf{e}_i \mathbf{e}_i^\mathsf{T}}_{\mathbf{U}_i}$
  - $\mathbf{U}_i = \mathbf{e}_i \mathbf{e}_i^\mathsf{T}$ – the $m \times m$ matrix: $\mathbf{U}_i \mathbf{e}_j = \mathbf{0}$

Example for the 3×3 matrix:

$$\begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} \Rightarrow \begin{vmatrix} -\lambda & 1 & 1 \\ 1 & -\lambda & 1 \\ 1 & 1 & -\lambda \end{vmatrix} \Rightarrow p(\lambda) = \lambda^3 - 3\lambda - 2 = 0 \Rightarrow \lambda_1 = 2;$$

$$\lambda_2 = \lambda_3 = -1 \Rightarrow \mathbf{e}_1 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}; \ \mathbf{e}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}; \ \mathbf{e}_3 = \frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ 2 \\ -1 \end{bmatrix}$$

Review of Linear Algebra, continued

Outer product of an m-dimensional column vector $\mathbf{a}$ with an n-dimensional row vector $\mathbf{b}$ (i.e. the transposed column vector):

$$\mathbf{a}\mathbf{b}^{\mathsf{T}} \equiv \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} \begin{bmatrix} b_1 & b_2 & \ldots & b_n \end{bmatrix} = \begin{bmatrix} a_1 b_1 & a_1 b_2 & \ldots & a_1 b_n \\ a_2 b_1 & a_2 b_2 & \ldots & a_2 b_n \\ \vdots & \vdots & \ddots & \vdots \\ a_m b_1 & a_m b_2 & \ldots & a_m b_n \end{bmatrix}$$

- It is a simple example of the matrix-matrix product
- The $m \times 1$ matrix $\mathbf{a}$ is the m-dimensional vector-column
- The $1 \times n$ matrix $\mathbf{b}$ is the n-dimensional vector-row

Review of Linear Algebra, continued

- Range, $\mathrm{range}(\mathbf{A})$, or span of an $m \times n$ matrix $\mathbf{A}$
  - The set of vectors $\mathbf{y}$ such that $\mathbf{y} = \mathbf{A}\mathbf{x}$ for some $\mathbf{x} \in \mathbb{R}^n$
  - The column space of $\mathbf{A}$
    - The space of all linear combinations of the columns of $\mathbf{A}$
- Nullspace, $\mathrm{null}(\mathbf{A})$, of an $m \times n$ matrix $\mathbf{A}$
  - The set of vectors $\mathbf{x}$, such that $\mathbf{A}\mathbf{x} = \mathbf{0} \in \mathbb{R}^m$
- Rank, $\mathrm{rank}(\mathbf{A})$, of an $m \times n$ matrix $\mathbf{A}$ – the dimension of the range, or column space, of $\mathbf{A}$
  - The column and row spaces of $\mathbf{A}$ are of the same dimension $\mathrm{rank}(\mathbf{A})$
  - $\mathrm{rank}(\mathbf{A}) \leq \min\{m, n\}$
  - A full rank $\mathbf{A}$ with $m \geq n$ has n linearly independent columns, which form a basis for $\mathrm{range}(\mathbf{A})$

Systems of Linear Equations

$$\begin{cases} 4x_1 + x_2 + 2x_3 = 24 \\ 2x_1 - x_2 - 2x_3 = -6 \\ -x_1 + 2x_2 - x_3 = -4 \end{cases} \Longrightarrow \begin{cases} x_1 = 3 \\ x_2 = 2 \\ x_3 = 5 \end{cases}$$

Given $m \times n$ matrix $\mathbf{A}$ and m-vector $\mathbf{b}$, find unknown n-vector $\mathbf{x}$ satisfying $\mathbf{Ax} = \mathbf{b}$

- Components of solution $\mathbf{x}$: coefficients of linear combination of columns of $\mathbf{A}$ representing $\mathbf{b}$
- $m \times m$ (or square) matrix $\mathbf{A}$ (m equations with m unknowns)
  - Underdetermined linear system: $m > n$ (less equations, than unknowns)
  - Overdetermined linear system: $m < n$ (more equations, than unknowns)

Systems of Linear Equations, continued

- Nonsingular matrix $\mathbf{A}$: (*i*) inverse matrix $\mathbf{A}^{-1}$ exists; or
  (*ii*) $\det(\mathbf{A}) \neq 0$; or
  (*iii*) $\text{rank}(\mathbf{A}) = m$, or
  (*iv*) $\mathbf{Ax} \neq \mathbf{0}$ for any vector $\mathbf{x} \neq \mathbf{0}$, or
  (*v*) $\text{range}(\mathbf{A}) = \mathbb{R}^m$, or
  (*vi*) $\text{null}(\mathbf{A}) = \{\mathbf{0}\}$
- Nonsingular $\mathbf{A}$ and arbitrary $\mathbf{b}$ – one unique solution $\mathbf{x}$

$$\begin{bmatrix} 2 & 3 \\ 5 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 8 \\ 13 \end{bmatrix} \Rightarrow \begin{matrix} 2x_1 + 3x_2 = 8 \\ 5x_1 + 4x_2 = 13 \end{matrix} \Rightarrow \begin{bmatrix} x_1 = 1 \\ x_2 = 2 \end{bmatrix}$$

- Singular $\mathbf{A}$ - infinitely many or none solutions, depending on $\mathbf{b}$

$$\underbrace{\begin{bmatrix} 2 & 3 \\ 4 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 4 \\ 7 \end{bmatrix}}_{\text{no solution if } \mathbf{b} \notin \text{range}(\mathbf{A})}; \underbrace{= \begin{bmatrix} 4 \\ 8 \end{bmatrix} \Rightarrow \mathbf{x} = \begin{bmatrix} \gamma \\ \frac{2}{3}(2-\gamma) \end{bmatrix} \text{ for any real } \gamma}_{\text{infinitely many solutions if } \mathbf{b} \in \text{range}(\mathbf{A})}$$

Forming a Simpler System with the Same Solution

- *Premultiplying* (from left) both sides of $\mathbf{Ax} = \mathbf{b}$ by any nonsingular matrix $\mathbf{M}$ does not affect solution:

$$\mathbf{MAx} = \mathbf{Mb} \Rightarrow \mathbf{x} = (\mathbf{MA})^{-1}\mathbf{Mb} = \mathbf{A}^{-1}\mathbf{M}^{-1}\mathbf{Mb} = \mathbf{A}^{-1}\mathbf{b}$$

- **Gaussian elimination** – transforming general system sequentially into **upper triangular form** using linear combinations of rows

$$\overbrace{\begin{bmatrix} 3 & 2 & 1 & 2 \\ 6 & 6 & 3 & 5 \\ 3 & 0 & 3 & 5 \\ 9 & 2 & 7 & 8 \end{bmatrix}}^{\mathbf{A}} \overbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}}^{\mathbf{x}} = \overbrace{\begin{bmatrix} 4 \\ 5 \\ 5 \\ 10 \end{bmatrix}}^{\mathbf{b}} \Rightarrow$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 & 1 & 2 \\ 6 & 6 & 3 & 5 \\ 3 & 0 & 3 & 5 \\ 9 & 2 & 7 & 8 \end{bmatrix}}_{\text{Eliminating the first column: } \mathbf{M}_1\mathbf{A}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ 5 \\ 5 \\ 10 \end{bmatrix}}_{\mathbf{M}_1\mathbf{b}}$$

Gaussian Elimination

Elimination for the first column (assuming $A_{11} \neq 0$) – zero components of the first column of the transformed matrix $\mathbf{B} = \mathbf{M}_1\mathbf{A}$, except of $B_{11} \equiv A_{11}$:

$$\overbrace{\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ -\frac{A_{21}}{A_{11}} & 1 & 0 & \dots & 0 \\ -\frac{A_{31}}{A_{11}} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{A_{n1}}{A_{11}} & 0 & 0 & \dots & 1 \end{bmatrix}}^{\mathbf{M}_1} \overbrace{\begin{bmatrix} A_{11} & A_{12} & A_{13} & \dots & A_{1n} \\ A_{21} & A_{22} & A_{23} & \dots & A_{2n} \\ A_{31} & A_{32} & A_{33} & \dots & A_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & A_{n3} & \dots & A_{nn} \end{bmatrix}}^{\mathbf{A}} =$$

$$\overbrace{\begin{bmatrix} A_{11} & A_{12} & A_{13} & \dots & A_{1n} \\ -\frac{A_{21}}{A_{11}}A_{11} + A_{21} = 0 & -\frac{A_{21}}{A_{11}}A_{12} + A_{22} & -\frac{A_{21}}{A_{11}}A_{13} + A_{23} & \dots & -\frac{A_{21}}{A_{11}}A_{1n} + A_{2n} \\ -\frac{A_{31}}{A_{11}}A_{11} + A_{31} = 0 & -\frac{A_{31}}{A_{11}}A_{12} + A_{32} & -\frac{A_{31}}{A_{11}}A_{13} + A_{33} & \dots & -\frac{A_{31}}{A_{11}}A_{1n} + A_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{A_{n1}}{A_{11}}A_{11} + A_{n1} = 0 & -\frac{A_{n1}}{A_{11}}A_{12} + A_{n2} & -\frac{A_{n1}}{A_{11}}A_{13} + A_{n3} & \dots & -\frac{A_{n1}}{A_{11}}A_{1n} + A_{nn} \end{bmatrix}}^{\mathbf{B}=\mathbf{M}_1\mathbf{A}}$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 & 1 & 2 \\ 6 & 6 & 3 & 5 \\ 3 & 0 & 3 & 5 \\ 9 & 2 & 7 & 8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}}_{\mathbf{M}_1 \mathbf{A} \mathbf{x}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ 5 \\ 5 \\ 10 \end{bmatrix}}_{\mathbf{M}_1 \mathbf{b}}$$

$$\begin{bmatrix} 3 & 2 & 1 & 2 \\ 0 & 2 & 1 & 1 \\ 0 & -2 & 2 & 3 \\ 0 & -4 & 4 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 4 \\ -3 \\ 1 \\ -2 \end{bmatrix} \Rightarrow$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 & 1 & 2 \\ 0 & 2 & 1 & 1 \\ 0 & -2 & 2 & 3 \\ 0 & -4 & 4 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}}_{\mathbf{M}_2 \mathbf{M}_1 \mathbf{A} \mathbf{x}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ -3 \\ 1 \\ -2 \end{bmatrix}}_{\mathbf{M}_2 \mathbf{M}_1 \mathbf{b}}$$

$$\begin{bmatrix} 3 & 2 & 1 & 2 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & 3 & 4 \\ 0 & 0 & 6 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 4 \\ -3 \\ -2 \\ -8 \end{bmatrix} \Rightarrow$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -2 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 & 1 & 2 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & 3 & 4 \\ 0 & 0 & 6 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}}_{\mathbf{M}_3 \mathbf{M}_2 \mathbf{M}_1 \mathbf{A} \mathbf{x}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -2 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ -3 \\ -2 \\ -8 \end{bmatrix}}_{\mathbf{M}_3 \mathbf{M}_2 \mathbf{M}_1 \mathbf{b}}$$

$$\begin{bmatrix} 3 & 2 & 1 & 2 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & 3 & 4 \\ 0 & 0 & 0 & -4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 4 \\ -3 \\ -2 \\ -4 \end{bmatrix}$$

Gaussian Elimination: Pivot Selection

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \Longrightarrow \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix} \Longrightarrow \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix} \Longrightarrow \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & * & * \end{bmatrix} \Longrightarrow \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & & * \end{bmatrix}$$

- Gaussian elimination as described in previous slides assumes that each current pivot $\widehat{A}_{ii} \neq 0$ at each step $i = 1, \ldots, n$
- If $\widehat{A}_{ii} = 0$, the remaining bottom rows $j = i+1, \ldots, n$ have to be permuted in order to get the non-zero pivot
- [Example by R. Sedgewick] Can the system $\begin{cases} 0 \cdot x_1 + 3x_2 & = & 6 \\ 5 \cdot x_1 + 0 \cdot x_2 & = & 5 \end{cases}$ be solved by Gaussian elimination without permuting the rows?
- For a non-singular matrix $\mathbf{A}$ such a permutation always exists
- The permutations have to be traced in order to restore at the end the initial order of the solution components.

Back-Substitution for Gaussian Elimination

To solve the resulting upper triangular system $\mathbf{C}\mathbf{x} = \mathbf{c}$:

$$\underbrace{\mathbf{M}_{n-1}\ldots\mathbf{M}_2\mathbf{M}_1\mathbf{A}}_{\mathbf{C}}\,\mathbf{x} = \underbrace{\mathbf{M}_{n-1}\ldots\mathbf{M}_2\mathbf{M}_1\mathbf{b}}_{\mathbf{c}}$$

– loop backwards, from n to 1:

$$\begin{cases} x_n = \frac{c_n}{C_{nn}} \\ x_i = \frac{1}{C_{ii}}\left(c_i - C_{i,i+1}x_{i+1} - \ldots - C_{i,n}x_n\right); \quad i = n-1, \ldots, 1 \end{cases}$$

For the example with $n = 4$ in Slides 27, 28, and 29:

$$\begin{aligned} x_4 &= \tfrac{-4}{-4} &&= 1 \\ x_3 &= \tfrac{1}{3}\left(-2 - 4 \cdot 1\right) &&= -2 \\ x_2 &= \tfrac{1}{2}\left(-3 - 1 \cdot (-2) - 1 \cdot 1\right) &&= -1 \\ x_1 &= \tfrac{1}{3}\left(4 - 2 \cdot (-1) - 1 \cdot (-2) - 2 \cdot 1\right) &&= 2 \end{aligned}$$

How to write numerical linear algebra software?

Don't !!!

Whenever possible, rely on existing, mature software libraries, e.g. LAPACK/LINPACK, BLAS, ATLAS, Boost uBlas, ...

- You can focus on the higher-level algorithm
- Your code will be more portable, less buggy, and will run faster — sometimes much faster!