Computational Astrophysics I: Introduction and basic concepts

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Matrices and Linear Algebra

Methods to solve matrix problems (e.g., inversion) useful for ODEs and PDEs, e.g., eigenvalue problem or radiative transfer with Feautrier scheme

Example: Vibrational spectrum of a molecule 1

n degrees of vibrational freedom $\rightarrow$ potential energy

$$U(q_1, q_2, \ldots, q_n) \simeq \frac{1}{2} \sum_{j,k}^{n} A_{jk} q_j q_k \tag{1}$$

in generalized coordinates around equilibrium state up to 2nd order term, coupling/potential parameter A_{jk} (e.g., spring constant).
Kinetic energy with generalized mass M_{jk}

$$T(\dot{q}_1, \dot{q}_2, \ldots, \dot{q}_n) \simeq \frac{1}{2} \sum_{j,k}^{n} M_{jk} \dot{q}_j \dot{q}_k \tag{2}$$

Example: Vibrational spectrum of a molecule 2

Apply Lagrange equation of 2nd kind

$$\frac{\partial \mathcal{L}}{\partial q_j} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_j} = 0 \qquad \text{with } \mathcal{L} = T - U \tag{3}$$

$$\text{Hence, equations of motion, for } k = 1, \ldots, n\text{: } \sum_{j=1}^{n}(A_{jk} q_j + M_{jk}\ddot{q}_j) = 0 \tag{4}$$

Assume an oscillatory motion $q_j = x_j\, e^{\imath\omega t} \rightarrow \frac{d^2}{dt^2}(x_j\, e^{\imath\omega t}) = -x_j\omega^2\, e^{\imath\omega t}$

$$\rightarrow \sum_{j=1}^{n}(A_{jk} - M_{jk}\omega^2)x_j = 0 \quad \text{or with } k = 1, \ldots, n \;:\quad \boldsymbol{A}\boldsymbol{x} = \omega^2 \boldsymbol{M}\boldsymbol{x} \tag{5}$$

set of linear homogenous equations. Nontrivial solution $\rightarrow$ determinant of coefficient matrix $\stackrel{!}{=} 0$
$\rightarrow \omega_k = \sqrt{\lambda_k}$ $(k = 1, \ldots, n)$ from equation

$$\det(\boldsymbol{A} - \lambda \boldsymbol{M}) = 0 \tag{6}$$

Matrix $\boldsymbol{A}$ with elements A_{ij} and $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n \rightarrow m \times n$ matrix.

$$\begin{array}{c} \\ m \\ \text{rows} \\ \downarrow \end{array} \begin{array}{c} n \text{ columns} \rightarrow \\ \begin{pmatrix} A_{11} & A_{12} & \ldots & A_{1n} \\ A_{21} & \ldots & & \\ \ldots & & & \\ A_{m1} & & & A_{mn} \end{pmatrix} \end{array}$$

If $m = n \rightarrow$ square matrix

Remember: Computer stores array in memory sequentially (1d), for C/C++ stored by rows (last index runs first)

$$A_{11}, A_{12}, \ldots, A_{1n}, A_{21}, \ldots, A_{mn} \tag{7}$$

whereas for Fortran stored by column (first index runs first):

$$A_{11}, A_{21}, \ldots, A_{m1}, A_{12}, \ldots, A_{mn} \tag{8}$$

Variable array $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$: $n \times 1$ matrix. Hence set of linear equations for $i = 1, 2, \ldots, n$, where x_i is unknown:

$$A_{i1}\, x_1 + A_{i2}\, x_2 + \ldots + A_{in}\, x_n = b_i \tag{9}$$

with coefficients A_{ij} and constants b_i, so express Eq. (9) in matrix form

$$\boldsymbol{A}\, \boldsymbol{x} = \boldsymbol{b} \tag{10}$$

with $\boldsymbol{A}\, \boldsymbol{x}$ from standard matrix multiplication for $\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$, i.e.

$$C_{ij} = \sum_k A_{ik} B_{kj} \tag{11}$$

(number of columns of $\boldsymbol{A} \stackrel{!}{=}$ number of rows of $\boldsymbol{B}$)

Example: Population numbers from statistical equilibrium (non-LTE)

"inflow" to level n_j (from all other levels) balanced by "outflow" from level n_j (to all other levels)

$$\sum_{\substack{i=1 \\ i\neq j}}^{N} n_i P_{ij} = \sum_{\substack{i=1 \\ i\neq j}}^{N} n_j P_{ji} \quad \forall\, j = 1, \ldots, N \tag{12}$$

$$\boldsymbol{n}\,\boldsymbol{P} = 0 \quad \text{with } P_{ii} := -\sum_{j\neq i} P_{ij} \tag{13}$$

Remember definitions: Inverse of a matrix $\boldsymbol{A}$ is $\boldsymbol{A}^{-1}$:

$$\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I} \tag{14}$$

with $I_{ij} = \delta_{ij}$.
The transpose of a matrix $\boldsymbol{A}^T$ is with column and row indices of $\boldsymbol{A}$ interchanged

$$A^T_{ij} = A_{ji} \tag{15}$$

Matrix operations IV

Trace of $\boldsymbol{A}$ ($\mathrm{Tr}\,\boldsymbol{A}$) is summation of diagonal elements of $\boldsymbol{A}$

$$\mathrm{Tr}\,\boldsymbol{A} = \sum_{i=1}^{n} A_{ii} \tag{16}$$

The determinant of square matrix $\boldsymbol{A}$

$$\det(\boldsymbol{A}) = \sum_{i=1}^{n} (-1)^{i+j} A_{ij} \det(\boldsymbol{R}_{ij}) \tag{17}$$

where $\boldsymbol{R}_{ij}$ is residual matrix of $\boldsymbol{A}$ with ith row and jth column removed ($\rightarrow$ recursive computation)

$$\text{e.g., } \det \begin{pmatrix} A_{11} & A12 \\ A_{21} & A_{22} \end{pmatrix} = A_{11}A_{22} - A_{12}A_{21} \tag{18}$$

Matrix operations V

Important properties of the determinant:

- Determinant of a 1×1 matrix = element itself.
- Determinant of a triangular matrix (lower or upper) is the product of diagonal elements: $\det(\boldsymbol{A}) = \prod_{i=1}^{n} A_{ii}$
- $\det(\boldsymbol{BA}) = \det(\boldsymbol{B}) \cdot \det(\boldsymbol{A})$ (if both $n \times n$)
- $\det(\boldsymbol{A}^{-1}) = \frac{1}{\det(\boldsymbol{A})}$ $\rightarrow$ integer entries for $\boldsymbol{A}$ and $\boldsymbol{A}^{-1} \Leftrightarrow \det(\boldsymbol{A}) = \pm 1$
- $\det(\boldsymbol{A}^{T}) = \det(\boldsymbol{A})$
- The determinant is an *n-linear function* of the n columns (rows). It is moreover an *alternating form*. Together with $\det(\boldsymbol{A}^{T}) = \det(\boldsymbol{A})$, this means:
  Interchanging any pair of columns or rows of a matrix multiplies its determinant by -1.

Inverse of $\boldsymbol{A}$ via (Cramer's rule)

$$A_{ij}^{-1} = (-1)^{i+j} \frac{\det(\boldsymbol{R}_{ij})}{\det(\boldsymbol{A})} \tag{19}$$

$\rightarrow$ if $\boldsymbol{A}^{-1}$ exists or $\det(\boldsymbol{A}) \neq 0$ $\rightarrow$ nonsingular matrix, singular otherwise ().

Examples for singular / non-singular (=regular) matrices:

- the matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix} \tag{20}$$

is non-singular, its determinant is $\det(\boldsymbol{A}) = -1$ and its inverse is

$$\boldsymbol{A}^{-1} = \begin{pmatrix} -3 & 2 \\ 2 & -1 \end{pmatrix} \tag{21}$$

- the matrix

$$\boldsymbol{B} = \begin{pmatrix} 1 & 2 \\ 0 & 0 \end{pmatrix} \tag{22}$$

is singular, its determinant is $\det(\boldsymbol{A}) = 0$ and there exists no inverse

$$\boldsymbol{B} \cdot \boldsymbol{M} = \begin{pmatrix} 1 & 2 \\ 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1a + 2c & 1b + 2d \\ 0 & 0 \end{pmatrix} \neq \boldsymbol{I} \tag{23}$$

- the matrix

$$\boldsymbol{C} = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix} \tag{24}$$

is singular, its determinant is $\det(\boldsymbol{A}) = 0$, as two of its lines are linearly dependent

Moreover, it can be useful to perform the following transformations, represented by a matrix multiplications : $\boldsymbol{A}' = \boldsymbol{M}\boldsymbol{A}$

1. interchanging two rows i and j, elements: $M_{ij} = 1; M_{ji} = 1; M_{kk} = 1$ for $k \neq i, j$ other elements $= 0 \rightarrow \det(\boldsymbol{M}\,\boldsymbol{A}) = -\det(\boldsymbol{A})$
2. multiply one row by λ: $M_{kk} = 1$ for $k \neq i$; $M_{ii} = \lambda \neq 0$, all other elements $= 0$ $\rightarrow \det(\boldsymbol{M}\,\boldsymbol{A}) = \det(\boldsymbol{M})\det(\boldsymbol{A}) = \lambda \det(\boldsymbol{A})$
3. add a row (or column) to another row (or column) multiplied by a factor λ: $M_{ii} = 1,\ M_{ij} = \lambda,\ M_{kl} = 0$. This can be also be written as

$$A'_{ij} = A_{ij} + \lambda A_{kj} \qquad \text{for } j = 1, 2, \ldots, n \tag{25}$$

and i and k are row indices, which can be the same. The determinant is preserved $\det(\boldsymbol{A}') = \det(\boldsymbol{A})$.

$\rightarrow$ see below for Gaussian elimination and matrix decomposition

The matrix eigenvalue problem is for a given matrix $\boldsymbol{A}$

$$\boldsymbol{A}\,\boldsymbol{x} = \lambda \boldsymbol{x} \tag{26}$$

with eigenvector $\boldsymbol{x}$ and corresponding eigenvalue λ of the matrix.
Also for the example of the vibrating molecules:

$$\boldsymbol{A}\boldsymbol{x} = \omega^2 \boldsymbol{M}\boldsymbol{x} \quad | \quad \boldsymbol{B} := \boldsymbol{M}^{-1}\boldsymbol{A} \tag{27}$$

$$\rightarrow \boldsymbol{B}\boldsymbol{x} = \omega^2 \boldsymbol{x} \tag{28}$$

→ Matrix eigenvalue problem = linear equation set problem
→ e.g., iterative solution

$$\boldsymbol{A}\,\boldsymbol{x}_{n+1} = \lambda_n \boldsymbol{x}_n \tag{29}$$

Moreover, the eigenvalues are preserved under a similarity transformation with a non-singular matrix $\boldsymbol{S}$

$$\boldsymbol{B} = \boldsymbol{S}^{-1}\boldsymbol{A}\boldsymbol{S} \tag{30}$$

$$\rightarrow\ \boldsymbol{B}\,\boldsymbol{y} = \lambda \boldsymbol{y} \quad \Leftrightarrow \quad \boldsymbol{A}\,\boldsymbol{x} = \lambda \boldsymbol{x} \qquad \text{for } \boldsymbol{x} = \boldsymbol{S}\boldsymbol{y} \tag{31}$$

$$\rightarrow\ \det(\boldsymbol{B}) = \det(\boldsymbol{A}) = \prod_{i=1}^{n} \lambda_i \tag{32}$$

→ computation of eigenvalues & eigenvectors usually complicated ...

The general problem:

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \tag{33}$$

where matrix $\boldsymbol{A}$ and vector $\boldsymbol{b}$ given and vector $\boldsymbol{x}$ unknown.

Straightforward solutions:

- Cramer's rule:

$$x_i = \frac{\det(\boldsymbol{A}_i)}{\det(\boldsymbol{A})} \tag{34}$$

where in $\boldsymbol{A}_i$ the i-th column is replaced by $\boldsymbol{b}$
$\rightarrow$ for a system of n equations: need to compute $n+1$ determinants, each of order n (see above), i.e., compute $n!$ terms each with $(n-1)$ multiplications
$\rightarrow (n+1) \times n! \times (n-1)$ multiplications,
e.g., for $n = 20 \rightarrow 10^{21}$ multiplications and for a computer with, e.g., 10 TFLOPS
$\rightarrow t \approx 3\,\text{a}$ only for multiplications (also note large accumulation of roundoff error)

- find the inverse $\boldsymbol{A}^{-1}$

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b} \tag{35}$$

$\rightarrow$ also time-consuming and instable, e.g., ($n = 1$, float)

$$7x = 21 \tag{36}$$

$$x = \frac{21}{7} = 3 \quad \text{(direct division)} \tag{37}$$

$$x = (7^{-1})(21) \quad \text{(compute inverse)} \tag{38}$$

$$= (.142857)(21) = 2.999997 \quad \text{(less accurate)} \tag{39}$$

computation of the inverse, e.g., via Cramer's rule (see above) or

with *Gauß-Jordan elimination* (see below) for system $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I}$:

$$\begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \cdot \begin{pmatrix} \hat{a}_{11} & \dots & \hat{a}_{1n} \\ \vdots & & \vdots \\ \hat{a}_{n1} & \dots & \hat{a}_{nn} \end{pmatrix} = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix} \tag{40}$$

hence, the j-th column of the inverse $\hat{a}_j = (\hat{a}_{1j}, \hat{a}_{2j}, \dots, \hat{a}_{nj})^T$ is solution of the system of linear equations

$$A \cdot \hat{a}_j = e_j \tag{41}$$

These equations are solved simultaneously by extending matrix $\boldsymbol{A}$ with $\boldsymbol{I}$:

$$(\, A \,|\, I \,) = \left(\begin{array}{ccc|ccc} a_{11} & \dots & a_{1n} & 1 & & 0 \\ \vdots & & \vdots & & \ddots & \\ a_{n1} & \dots & a_{nn} & 0 & & 1 \end{array} \right) \tag{42}$$

$\rightarrow$ elementary row operations $\rightarrow$ matrix $\boldsymbol{A}$ into upper triangular form (forward elimination)

$$(\,D\,|\,B\,) = \left(\begin{array}{ccc|ccc} * & \dots & * & * & \dots & * \\ & \ddots & \vdots & \vdots & & \vdots \\ 0 & & * & * & \dots & * \end{array}\right) \tag{43}$$

$\rightarrow$ if no zeros on diagonal $\rightarrow$ invertible, bring into diagonal form:

$$(\,I\,|\,A^{-1}\,) = \left(\begin{array}{ccc|ccc} 1 & & 0 & \hat{a}_{11} & \dots & \hat{a}_{1n} \\ & \ddots & & \vdots & & \vdots \\ 0 & & 1 & \hat{a}_{n1} & \dots & \hat{a}_{nn} \end{array}\right) \tag{44}$$

or compute inverse with *characteristic polynomial*:

$$A^{-1} = \frac{-1}{\det(A)}\left(\alpha_1 I_n + \alpha_2 A + \ldots + \alpha_n A^{n-1}\right) \tag{45}$$

where the coefficients of the chracteristical polynomial of $\boldsymbol{A}$ can be obtained from $\chi(t) = \det(t\boldsymbol{I} - \boldsymbol{A}) = \alpha_0 + \alpha_1 \cdot t^1 + \ldots + \alpha_n \cdot t^n$

Matrix problems can be easily solved for an upper (lower) triangular matrix, for which elements below (above) the diagonal = 0,

$$\begin{pmatrix} R_{11} & R_{12} & \dots & R_{1n} \\ 0 & R_{22} & \dots & R_{2n} \\ & & \ddots & \\ 0 & 0 & \dots & R_{nn} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \dots \\ c_n \end{pmatrix} \tag{46}$$

via backward (forward) substitution, i.e. starting with $x_n = c_n/R_{nn}$ and

$$x_i = \frac{c_i - \sum_{j=i+1}^{n} R_{ij} x_j}{R_{ii}} \qquad \text{for } i = n-1, \dots, 1 \tag{47}$$

$\rightarrow$ need algorithms for transformation into triangular form

Gaussian elimination

1. *Forward elimination:* Transform linear equation set $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ by a sequence of matrix operations j from original matrix $\boldsymbol{A} = \boldsymbol{A}^{(0)}$ to $\boldsymbol{A}^{(j)}$, hence after $n-1$ steps for a $n \times n$ matrix

$$\boldsymbol{A}^{(n-1)}\boldsymbol{x} = \boldsymbol{b}^{(n-1)} \tag{48}$$

where $A_{ij}^{(n-1)} = 0$ for $i > j$:

1. multiply 1st equation (1st row $\boldsymbol{A}$ and $b_1^{(0)}$) by $-A_{i1}^{(0)}/A_{11}^{(0)}$ and add to ith equation (row) for $i > 1 \rightarrow$ 1st element of every row except 1st row eliminated $\rightarrow \boldsymbol{A}^{(1)}$
2. multiply 2nd equation by $-A_{i2}^{(1)}/A_{22}^{(1)}$ and add to ith equation for $i > 2 \rightarrow$ 2nd element of every row except 1st & 2nd row eliminated $\rightarrow \boldsymbol{A}^{(2)}$
3. ...
4. upper triangular matrix $\boldsymbol{A}^{(n-1)}$

2. *backward substitution* according to Eq. (47)

Gaussian elimination III

ad 1.: all diagonal elements A_{jj} are used in denominators $-A_{ij}^{(j-1)}/A_{jj}{}^{(j-1)}$
$\rightarrow$ problems if diagonal elements $= 0$ or ≈ 0
Solution: pivoting (from french pivot=center of rotation) $\rightarrow$ interchange rows/columns to put always largest (absolut value) element on diagonal
full pivoting: interchange columns and rows, need to keep track of order ...
partial pivoting: only search for pivot in remaining elements of the current column (swap rows only)
$\rightarrow$ partial pivoting usually good compromise between speed and accuracy
$\rightarrow$ use index to record order of pivot elements instead of physically interchanging
$\rightarrow$ *rescaling*: rescale all elements from a row by its largest element before comparing to find pivot (reduces rounding errors)

Example: Gaussian elimination in Fortran - code sniplet

```
! partial pivot. Gaussian elimin.
DIMENSION A(N,N),INDX(N),C(N)
DO I = 1, N
 INDX(I) = I ! init. index
 C1 = 0.0
 DO J = 1, N ! rescale coeff.
  C1 = AMAX1(C1,ABS(A(I,J)))
 ENDDO
 C(I) = C1
ENDDO

DO J = 1, N-1 ! search pivots
 PI1 = 0.0
 DO I = J, N
  PI = ABS(A(INDX(I),J)) / C(INDX(I))
  IF (PI.GT.PI1) THEN
   PI1 = PI
   K   = I
  ENDIF
 ENDDO
 ITMP = INDX(J)
 INDX(J) = INDX(K)
 INDX(K) = ITMP
 DO I = J + 1, N ! elimin. subdiagonal
  PJ = A(INDX(I),J) / A(INDX(J),J)
  A(INDX(I),J) = PJ
  DO L = J + 1, N
   A(INDX(I),L) = A(INDX(I),L) - &
   PJ * A(INDX(J),L)
  ENDDO
 ENDDO
ENDDO
```

Example: Gaussian elimination by hand I

$$\begin{pmatrix} 10 & -7 & 0 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 4 \\ 6 \end{pmatrix} \tag{49}$$

1.) eliminate x_1 from row 2 & 3 $\rightarrow$ add $3/10 = 0.3\times$ 1st row to 2nd row & add $-5/10 = -0.5\times$ 1st row to 3rd row:

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & -0.1 & 6 \\ 0 & 2.5 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 6.1 \\ 2.5 \end{pmatrix} \tag{50}$$

2.) eliminate x_2 from row 3 $\rightarrow$ a) pivoting: interchange row 2 & 3 so that coefficient of x_2 in row 2 is largest (because of roundoff errors $\rightarrow$ only for computers necessary)

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & -0.1 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 2.5 \\ 6.1 \end{pmatrix} \tag{51}$$

Example: Gaussian elimination by hand II

2.b) now add $0.1/2.5 = 0.04\times$ 2nd row to 3rd row:

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 2.5 \\ 6.2 \end{pmatrix} \tag{52}$$

Finally: backward substitution, starting with last row:

$$6.2\, x_3 = 6.2 \rightarrow x_3 = 1 \tag{53}$$

$$2.5\, x_2 + 5 \cdot 1 = 2.5 \rightarrow x_2 = -1 \tag{54}$$

$$10\, x_1 + (-7) \cdot (-1) + 0 = 7 \quad \rightarrow x_1 = 0 \tag{55}$$

This can be also expressed in matrix notation: Let

$$\boldsymbol{M}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0.3 & 1 & 0 \\ -0.5 & 0 & 1 \end{pmatrix} \rightarrow \boldsymbol{M}_1\boldsymbol{A} = \begin{pmatrix} 10 & -7 & 0 \\ 0 & -0.1 & 6 \\ 0 & 2.5 & 5 \end{pmatrix}, \quad \boldsymbol{M}_1\boldsymbol{b} = \begin{pmatrix} 7 \\ 6.1 \\ 2.5 \end{pmatrix} \tag{56}$$

Example: Gaussian elimination by hand III

Let then

$$\boldsymbol{P}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{M}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0.04 & 1 \end{pmatrix} \tag{57}$$

$$\rightarrow \boldsymbol{M}_2\boldsymbol{P}_2\boldsymbol{M}_1\boldsymbol{A} = \begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.2 \end{pmatrix} = \boldsymbol{U}, \quad \boldsymbol{M}_2\boldsymbol{P}_2\boldsymbol{M}_1\boldsymbol{b} = \begin{pmatrix} 7 \\ 2.5 \\ 6.2 \end{pmatrix} = \boldsymbol{c} \tag{58}$$

Hence $\boldsymbol{U}\boldsymbol{x} = \boldsymbol{c}$, with upper triangular matrix $\boldsymbol{U}$.
The matrices $\boldsymbol{P}_k, k = 1, \ldots, n-1$ are the permutations matrices, inferred from the identity matrix $\boldsymbol{I}$ by interchanging rows in same way as for $\boldsymbol{A}$ in the kth step, and $\boldsymbol{M}_k$ is multiplication matrix, inferred from identy matrix by inserting mulitpliers used in kth step below diagonal in kth column $\rightarrow \boldsymbol{M}_k$ are lower triangular matrices

$$\boldsymbol{M} := \boldsymbol{M}_{n-1}\boldsymbol{P}_{n-1} \ldots \boldsymbol{M}_1\boldsymbol{P}_1 \tag{59}$$

$$\boldsymbol{U} = \boldsymbol{M}\boldsymbol{A} \quad (\text{“triangular decomposition” of } \boldsymbol{A}) \tag{60}$$

LU decomposition I

More general approach: decompose *nonsingular* matrix $\boldsymbol{A}$ into two triangular matrices

$$\boldsymbol{A} = \boldsymbol{L}\,\boldsymbol{U} \tag{61}$$

with lower (left) triangular matrix $\boldsymbol{L}$ and upper (right) triangular matrix $\boldsymbol{U}$ (or $\boldsymbol{R}$), hence

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{L}\boldsymbol{U}\boldsymbol{x} = \boldsymbol{b} \tag{62}$$

$$\rightarrow \text{ first, solve 1. } \boldsymbol{L}\boldsymbol{y} = \boldsymbol{b} \rightarrow \boldsymbol{y} \tag{63}$$

$$\text{then 2. } \boldsymbol{U}\boldsymbol{x} = \boldsymbol{y} \rightarrow \boldsymbol{x} \tag{64}$$

i.e. once $\boldsymbol{A} = \boldsymbol{L}\,\boldsymbol{U}$ obtained $\rightarrow$ easy to solve for *any* b.
More general case: re-order matrix $\boldsymbol{A}$ by, e.g., row-permutations (partial pivoting):

$$\boldsymbol{P}\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}, \text{ then} \tag{65}$$

$$\boldsymbol{L}\boldsymbol{U}\boldsymbol{x} = \boldsymbol{P}\boldsymbol{b} \tag{66}$$

$$1.\ \boldsymbol{L}\boldsymbol{y} = \boldsymbol{P}\boldsymbol{b} \rightarrow \boldsymbol{y} \tag{67}$$

$$2.\ \boldsymbol{U}\boldsymbol{x} = \boldsymbol{y} \rightarrow \boldsymbol{x} \tag{68}$$

e.g. $\rightarrow$ Crout's method

start with $L_{i1} = A_{i1}$ and $U_{1j} = A_{1j}/A_{11}$, then recursively:

$$L_{ij} = A_{ij} - \sum_{k=1}^{j-1} L_{ik} U_{kj} \tag{69}$$

$$U_{ij} = \frac{1}{L_{ii}} \left(A_{ij} - \sum_{k=1}^{i-1} L_{ik} U_{kj} \right) \tag{70}$$

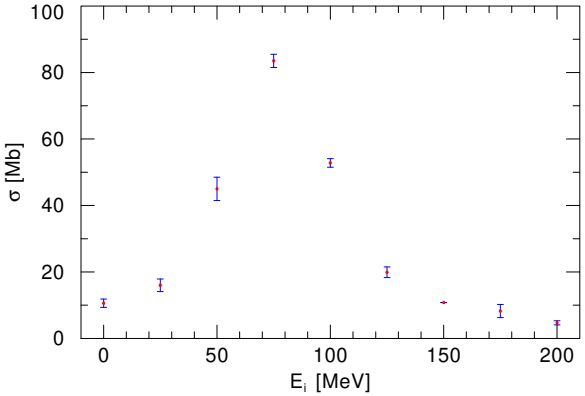
Usually no need to implement by yourself, instead use libraries, e.g., `LINPACK`:

- `DGEFA` performs LU decomposition by Gaussian elimination
- `DGESL` uses that decomposition to solve the given system of linear equations
- `DGEDI` uses decomposition to compute inverse of a matrix

Application: Interpolating data I

Remember following measurement of a cross section

E_i [MeV]	0	25	50	75	100	125	150	175	200
$\sigma(E_i)$ [Mb]	10.6	16.0	45.0	83.5	52.8	19.9	10.8	8.25	4.7
$\sigma_{\sigma(E_i)}$ [Mb]	1.26	1.9	3.5	2.0	1.3	1.6	0.04	1.96	0.61



The cross section can be described by Breit-Wigner formula

$$f(E) = \frac{f_r}{(E - E_r)^2 + \Gamma^2/4} \tag{71}$$

Interpolation problem

We want to determine $\sigma(E)$ for values of E which lie between measured values of E

By

- numerical interpolation (assumption of data representation by polynomial in E):
  $\rightarrow$ see previous lectures
  $\rightarrow$ ignores errors in measurement (noise)
- fitting parameters of an underlying model, e.g., Breit-Wigner with f_r, E_r, Γ, (taking errors into account), i.e., minimizing χ^2
- Fourier analysis (next semester lecture)

Already seen for linear regression:
We have N_D data points

$$(x_i, y_i \pm \sigma_i) \quad i = 1, \ldots, N_D \tag{72}$$

and a function $y = g(x)$ (=model) with parameters $\{a_m\}$; fit function to data, such that $\chi^2 = min$:

$$\chi^2 := \sum_{i=1}^{N_D} \left(\frac{y_i - g(x_i; \{a_m\})}{\sigma_i} \right)^2 \tag{73}$$

i.e. for M_P parameters $\{a_m, m = 1 \ldots M_P\}$

$$\frac{\partial \chi^2}{\partial a_m} \stackrel{!}{=} 0 \Rightarrow \sum_{i=1}^{N_D} \frac{[y_i - g(x_i)]}{\sigma_i^2} \frac{\partial g(x_i)}{\partial a_m} = 0 \quad (m = 1, \ldots, M_P) \tag{74}$$

$\rightarrow$ solve M_P equations, usually nonlinear in a_m

Least square fitting II

goodness of fit, assumptions

- deviations to model only due to random errors
- Gaussion distribution of errors

$\rightarrow$ then, fit is good when $\chi^2 \approx N_D - M_P$ (degrees of freedom)

- if $\chi^2 \ll N_D - M_P \rightarrow$ probably too many parameters or errors σ_i to large (fitting random scatter)
- if $\chi^2 \gg N_D - M_P \rightarrow$ model not good or underestimated errors or non-random errors

$\rightarrow$ for linear fit see above

Non-linear fit

remember Breit-Wigner resonance formula Eq. (71)

$$f(E) = \frac{f_r}{(E - E_r)^2 + \Gamma^2/4} \tag{75}$$

$\rightarrow$ determine f_r, E_r, Γ
$\rightarrow$ nonlinear equations in the parameters

$$a_1 = f_r \qquad a_2 = E_r \qquad a_3 = \Gamma^2/4 \tag{76}$$

$$\Rightarrow g(x) = \frac{a_1}{(x - a_2)^2 + a_3} \tag{77}$$

$$\frac{\partial g}{\partial a_1} = \frac{1}{(x - a_2)^2 + a_3}, \quad \frac{\partial g}{\partial a_2} = \frac{-2a_1(x - a_2)}{[(x - a_2)^2 + a_3]^2}, \quad \frac{\partial g}{\partial a_3} = \frac{-a_1}{[(x - a_2)^2 + a_3]^2} \tag{78}$$

Insert into Eq. (74):

$$\sum_{i=1}^{9} \frac{y_i - g(x_i, a)}{(x_i - a_2)^2 + a_3} = 0 \qquad \sum_{i=1}^{9} \frac{[y_i - g(x_i, a)](x_i - a_2)}{[(x_i - a_2)^2 + a_3]^2} = 0$$
$$\sum_{i=1}^{9} \frac{y_i - g(x_i, a)}{[(x_i - a_2)^2 + a_3]^2} = 0 \tag{79}$$

$\rightarrow$ *three* nonlinear equations for unknown a_1, a_2, a_3, i.e. cannot be solved by linear algebra but can be solved with help of Newton-Raphson method, i.e. find the roots for the equations above

$$f_i(a_1, \ldots, a_M) = 0 \qquad i = 1, \ldots, M \tag{80}$$

So

$$f_1(a_1, a_2, a_3) = \sum_{i=1}^{9} \frac{y_i - g(x_i, a)}{(x_i - a_2)^2 + a_3} = 0 \tag{81}$$

$$f_2(a_1, a_2, a_3) = \sum_{i=1}^{9} \frac{[y_i - g(x_i, a)](x_i - a_2)}{[(x_i - a_2)^2 + a_3]^2} = 0 \tag{82}$$

$$f_3(a_1, a_2, a_3) = \sum_{i=1}^{9} \frac{y_i - g(x_i, a)}{[(x_i - a_2)^2 + a_3]^2} = 0 \tag{83}$$

with intial guesses for a_1, a_2, a_3.

Newton-Raphson method for a system of nonlinear equations
Remember for 1dim Newton-Raphson method, correction for Δx:

$$f(x_0) + f'(x_0) \cdot \Delta x \stackrel{!}{=} 0 \tag{84}$$

$$\Delta x = -\frac{f(x_0)}{f'(x_0)} \tag{85}$$

For our system of equations $f_i(a_1, \ldots, a_M) = 0$, we assume that for our approximation (intial guess) $\{a_i\}$ corrections $\{\Delta x_i\}$ exist so that

$$f_i(a_1 + \Delta a_1, a_2 + \Delta a_2, a_3 + \Delta a_3) = 0 \qquad i = 1, 2, 3 \tag{86}$$

$\rightarrow$ linear approximation (two terms of Taylor series):

$$f_i(a_1 + \Delta a_1, \ldots) \simeq f_i(a_1, a_2, a_3) + \sum_{j=1}^{3} \frac{\partial f_i}{\partial a_j} \Delta a_j = 0 \qquad i = 1, 2, 3 \tag{87}$$

$\rightarrow$ set of 3 linear equations in 3 unknowns

as explicit equations:

$$f_1 + \partial f_1/\partial a_1 \Delta a_1 + \partial f_1/\partial a_2 \Delta a_2 + \partial f_1/\partial a_3 \Delta a_3 = 0 \quad (88)$$
$$f_2 + \partial f_2/\partial a_1 \Delta a_1 + \partial f_2/\partial a_2 \Delta a_2 + \partial f_2/\partial a_3 \Delta a_3 = 0 \quad (89)$$
$$f_3 + \partial f_3/\partial a_1 \Delta a_1 + \partial f_3/\partial a_2 \Delta a_2 + \partial f_3/\partial a_3 \Delta a_3 = 0 \quad (90)$$

Or as single matrix equation:

$$\begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix} + \begin{pmatrix} \partial f_1/\partial a_1 & \partial f_1/\partial a_2 & \partial f_1/\partial a_3 \\ \partial f_2/\partial a_1 & \partial f_2/\partial a_2 & \partial f_2/\partial a_3 \\ \partial f_3/\partial a_1 & \partial f_3/\partial a_2 & \partial f_3/\partial a_3 \end{pmatrix} \begin{pmatrix} \Delta a_1 \\ \Delta a_2 \\ \Delta a_3 \end{pmatrix} = 0 \quad (91)$$

Or in matrix notation

$$\mathrm{f} + \mathrm{F}' \, \boldsymbol{\Delta a} = 0 \Rightarrow \mathrm{F}' \, \boldsymbol{\Delta a} = -\boldsymbol{f} \quad (92)$$

Where we want to solve for $\boldsymbol{\Delta a}$ (the corrections)
Matrix $\boldsymbol{F}'$ sometimes written as $\boldsymbol{J}$ is called the *Jacobian* matrix (with entries $f'_{ij} = \partial f_i/\partial a_j$).

Equation $\boldsymbol{F}'\Delta a = -\boldsymbol{f}$ corresponds to standard form $\boldsymbol{Ax} = \boldsymbol{b}$ for systems of linear equations. Formally solution obtained by multiplying with inverse of $\boldsymbol{F}'$

$$\boldsymbol{\Delta a} = -\boldsymbol{F}'^{-1}\boldsymbol{f} \tag{93}$$

$\rightarrow$ inverse must exist for unique solution
$\rightarrow$ same form as for 1d Newton-Raphson: $\Delta x = -(1/f')f$
$\rightarrow$ iterate as for 1d Newton-Raphson till $\boldsymbol{f} \approx 0$

compute derivatives for the system numerically

$$f'_{ij} = \frac{\partial f_i}{\partial a_j} \simeq \frac{f_i(a_j + \Delta a_j) - f_i(a_j)}{\Delta a_j} \tag{94}$$

with Δa_j sufficiently small, e.g., 1% of a

Nonlinear fit with Newton-Raphson

In our nonlinear fit problem the Newton step

$$\mathrm{F}' \, \boldsymbol{\Delta a} = -\boldsymbol{f} \tag{95}$$

can be solved for $\boldsymbol{\Delta a}$ with help of `DGEFA` and `DGESL` (see p. 27):

```
CALL DGEFA(FPRIME, NDIM, NDIM, IPVT, INFO)
IF (INFO .NE. 0) STOP 'JACOBIAN MATRIX WITH 0 ON DIAGONAL'
CALL DGESL(FPRIME, NDIM, NDIM, IPVT, F)
```

where the solution $\boldsymbol{\Delta a}$ is written to vector `F`