Computational Physics
TU Dortmund - SuSe 2021

Solutions to exercise sheet 1

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April 22, 2021

0. Comprehension questions

0.1. What are the possibilities to solve systems of linear equations (with an unique solution)?

System of linear equations (SLE): $\boldsymbol{A}\vec{x} = \vec{b}$

- Calculate the inverse matrix $\Rightarrow \vec{x} = \boldsymbol{A}^{-1}\vec{b}$
- Gauß algorithm
- LU decomposition: $\boldsymbol{A} = \boldsymbol{P} \cdot \boldsymbol{L} \cdot \boldsymbol{U}$
  $\boldsymbol{L}$ is a lower triangular matrix and $\boldsymbol{U}$ is an upper triangular matrix.
  $\boldsymbol{P}$ is the "pivoting matrix" and satisfies $\boldsymbol{P}^T = \boldsymbol{P}^{-1}$.
  $\Rightarrow (\boldsymbol{P} \cdot \underbrace{(\boldsymbol{L} \cdot \overbrace{(\boldsymbol{U} \cdot \vec{x})}^{\vec{y}:=})}_{\vec{z}:=}) = \vec{b}$
  Then calculate $\vec{z} = \boldsymbol{P}^T \cdot \vec{b}$ and then solve the systems of linear equations:
  $\boldsymbol{L} \cdot \vec{y} = \vec{z}$ and $\boldsymbol{U} \cdot \vec{x} = \vec{y}$
- If the matrix $\boldsymbol{A}$ is not a square matrix, multiply the system of equations with $\boldsymbol{A}^T$ from the left.
  Now $\tilde{\boldsymbol{A}} := \boldsymbol{A}^T \cdot \boldsymbol{A}$ is a square matrix.

0.2. Why is a pivoting strategy necessary in general?

Pivoting reduces the effect of rounding errors. It reduces the amount of small to big number multiplications.

1. Change of basis with LU decomposition

Primitive lattice vectors:

$$\vec{a}_1 = \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix}; \qquad \vec{a}_2 = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix}; \qquad \vec{a}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{1}$$

1.a). What kind of crystal system is represented?

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1.b). Defect at $\vec{b} = (2, 0, 2)^T$

Coordinate transformation matrix to $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$:

$$\boldsymbol{A} = (\vec{a}_1, \vec{a}_2, \vec{a}_3) = \begin{pmatrix} 0.5 & -0.5 & 0 \\ 0.866 & 0.866 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2}$$

With the C++ module "Eigen::PartialPivLU" the LU decomposition yields

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3}$$

$$\boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 \\ 0.577 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4}$$

$$\text{and} \tag{5}$$

$$\boldsymbol{U} = \begin{pmatrix} 0.866 & 0.866 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{6}$$

Solving $\boldsymbol{A} \cdot \vec{x} = \vec{b}$ yields

$$\vec{x} = \begin{pmatrix} 2 \\ -2 \\ 2 \end{pmatrix}. \tag{7}$$

1.c). Defect at $\vec{c} = (1, 2\sqrt{3}, 3)^T$

You can reuse the LU decomposition which has a complexity of $O(N^3)$. You have to inversly solve the SLE which has a complexity of $O(N^2)$.

Solving $\boldsymbol{A} \cdot \vec{y} = \vec{c}$ yields

$$\vec{y} = \begin{pmatrix} 3 \\ 1 \\ 3 \end{pmatrix}. \tag{8}$$

1.d). LU decomposition for the basis $\{\vec{a}_3, \vec{a}_2, \vec{a}_1\}$

With the C++ module "Eigen::PartialPivLU" the LU decomposition of

$$\boldsymbol{A}_2 = (\vec{a}_3, \vec{a}_2, \vec{a}_1) = \begin{pmatrix} 0 & -0.5 & 0.5 \\ 0 & 0.866 & 0.866 \\ 1 & 0 & 0 \end{pmatrix} \tag{9}$$

yields

$$\boldsymbol{P}_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{10}$$

$$\boldsymbol{L}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.577 & 1 \end{pmatrix} \tag{11}$$

$$\boldsymbol{U}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.866 & 0.866 \\ 0 & 0 & 1 \end{pmatrix}. \tag{12}$$

The numeric values stay the same as in b) but the position of these values change their position.

1.e). How does the problem simplify when the primitive lattice vectors are pairwise orthogonal?

When the matrix $\boldsymbol{A}$ is orthogonal, its inverse is just the transposed matrix and the LU decomposition is not necessary. One can simply calculate $\vec{x} = \boldsymbol{A}^{-1} \cdot \vec{b}$.

2. Linear regression

Table 1: data points (x, y)

x	0	2.5	-6.3	4	-3.2	5.3	10.1	9.5	-5.4	12.7
y	4	4.3	-3.9	6.5	0.7	8.6	13	9.9	-3.6	15.1

2.a). Problem formulation & 2.b) Tranformation into a system with a square matrix

We want to calculate a linear regression in the form

$$y(x) = mx + n\,. \tag{13}$$

For this, a naiv approach would be to solve a SLE

$$\vec{y} = \underbrace{\begin{pmatrix} | & 1 \\ \vec{x} & \vdots \\ | & 1 \end{pmatrix}}_{\boldsymbol{A}:=} \underbrace{\begin{pmatrix} m \\ n \end{pmatrix}}_{\vec{m}:=}, \tag{14}$$

but this SLE probably has no solution. Instead we want to calculate the minimum of the quadratic error

$$R := \sum_i (\boldsymbol{A}\vec{m} - \vec{y})_i^2\,. \tag{15}$$

As shown in the lecture, this "least-square minimum" is calculated by solving

$$\underbrace{\boldsymbol{A}^T\boldsymbol{A}}_{\boldsymbol{P}:=}\,\vec{m} = \underbrace{\boldsymbol{A}^T\vec{y}}_{\vec{b}:=} \tag{16}$$

where $\boldsymbol{P}$ is a square matrix.

2.c). Carrying out the linear regression & 2.d) Plotting the linear regression

The given data points in Table 1 yield the following:

$$\boldsymbol{P} = \begin{pmatrix} 482.98 & 29.2 \\ 29.2 & 10 \end{pmatrix}$$

$$\vec{b} = \begin{pmatrix} 541.22 \\ 54.6 \end{pmatrix}$$

Now the LU decomposition of $\boldsymbol{P}$ yields

$$\begin{aligned}
\boldsymbol{P}_{LU} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
\boldsymbol{L} &= \begin{pmatrix} 1 & 0 \\ 0.060458 & 1 \end{pmatrix} \\
\boldsymbol{U} &= \begin{pmatrix} 482.98 & 29.2 \\ 0 & 8.23463 \end{pmatrix} .
\end{aligned}$$

And solving the SLE Equation 16 yields

$$\vec{m} = \begin{pmatrix} m \\ n \end{pmatrix} = \begin{pmatrix} 0.959951 \\ 2.65694 \end{pmatrix} . \tag{17}$$

The linear regression is plotted in Figure 1 using these parameters m and n.

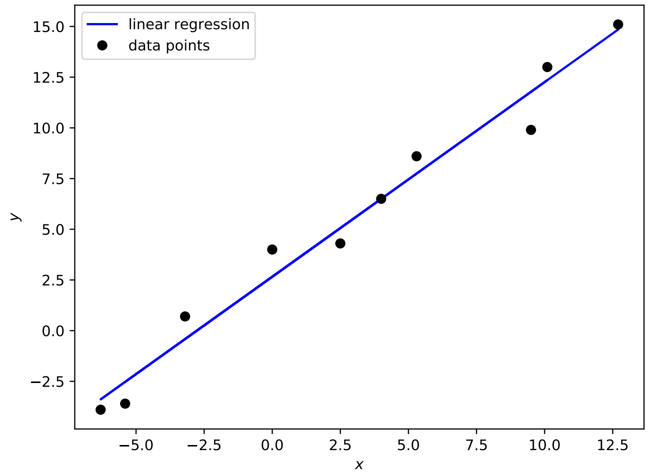

Figure 1: Plot of the linear regression