

## Linear Problems

Linear problems are about the vast majority of everyday problems. If one apple costs 10 cents, three apples will usually cost 30 cents. In other words: Linear problems deal with proportionality: double effort, double result.

For a single variable this is obvious, the solution of such proportionality problems is by “the rule of three”, in German “Dreisatz”. If there are more than one variables this becomes trickier. Example:

Three farmers altogether have produced 40 tons of corn. The amount of farmer X plus two times farmer Z would give 38 tons, one half farmer X plus one half farmer Y plus farmer Z would give 25 tons. How many tons has each farmer produced?

This can be cast into 3 equations:  $X+Y+Z = 40$ ;  $X+2*Z=38$ ;  $X/2+Y/2+Z=25$ .

In Matrix-Form:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} * \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 40 \\ 38 \\ 25 \end{pmatrix}$$

with  $a_{11}=a_{12}=a_{13}=1$ ;  $a_{21}=1, a_{22}=0, a_{23}=2$ ;  $a_{31}=1/2, a_{32}=1/2, a_{33}=1$ .

Of course this still can be simply solved by inserting e.g.  $X=38-2*Z$  into the other equations, to eliminate X and in the next step similarly eliminating Y, but for larger problems one prefers to use computers.

Such larger problems with ten thousands of variables occur by discretizing continuous problems such as hydrodynamic flow by a lattice-model. For these models algorithms like the Gauss-Seidel scheme are usually sufficient. But for sets of differential-equations such as the (linear!) Maxwell equations of electrodynamics (describing the propagation of light and radio-waves) the more general scheme of Eigenvalue-Eigenvector-analysis and matrix-diagonalization is preferable.

Formally, we may write the matrix-equation above as  $\mathbf{A} \mathbf{x} = \mathbf{b}$  with  $\mathbf{A}$  the matrix  $[=a_{11},a_{12},a_{13},\dots, \text{etc}]$ ,  $\mathbf{b}$  the vector on the right-hand-side  $[=40,38,25]$ , and  $\mathbf{x}$  the vector whose elements X,Y,Z are to be found. The Eigenvalue-Eigenvector-analysis tries to find the matrix  $\mathbf{T}$  of Eigenvectors (and its inverse  $=\mathbf{T}^{-1}$ ) which transforms  $\mathbf{A}$  into **diagonal form**  $\mathbf{\Lambda}$ , where only the diagonal elements are non-zero:

$$\mathbf{T} \mathbf{A} \mathbf{T}^{-1} \mathbf{T} \mathbf{x} = \mathbf{T} \mathbf{b} = \mathbf{\beta} \quad \text{or} \quad \mathbf{\Lambda} \mathbf{\xi} = \mathbf{\beta}, \quad \text{with} \quad \mathbf{\Lambda} = \mathbf{T} \mathbf{A} \mathbf{T}^{-1}, \quad \text{and} \quad \mathbf{\xi} = \mathbf{T} \mathbf{x} \text{ (unknown).}$$

Note that  $\mathbf{T}^{-1} \mathbf{T} = \mathbf{1}$  is the unit-matrix with only “1” on the main diagonal. This equation  $\mathbf{\Lambda} \mathbf{\xi} = \mathbf{\beta}$  is trivially resolved for vector  $\mathbf{\xi}$ , since there is only one element in each line of matrix  $\mathbf{\Lambda}$ . The final solution for  $\mathbf{x} [=X,Y,Z]$  is obtained by back-transforming  $\mathbf{\xi}$ :  $\mathbf{x} = \mathbf{T}^{-1} \mathbf{\xi}$ .

Below we first introduce the Eigenvalue-problem and then give a simple example for two variables.

# Eigenvalues: 2 x 2 Matrices

Linear Problems can be solved by Diagonalization.

We will formulate linear problems as Eigenvalue-problems. We start with a general  $2 \times 2$  matrix  $\mathbf{H} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ , where the elements a,b,c,d can be any complex numbers. The vector with the elements  $\begin{bmatrix} x \\ y \end{bmatrix}$  is the eigenvector, and  $\lambda$  stands for an Eigenvalue:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \quad (1)$$

Moving everything to the left hand side, one has the homogeneous system of linear equations

$$\begin{pmatrix} a - \lambda & b \\ c & d - \lambda \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \mathbf{0}. \quad (2)$$

This system has only non-trivial solutions  $x, y \neq 0$  when the determinant of the matrix is zero. The evaluation of the determinant leads to a polynom of 2-nd degree

$$\begin{aligned} (a - \lambda)(d - \lambda) - cb &= 0, \\ \lambda^2 - (a + d)\lambda + ad - cb &= 0. \end{aligned} \quad (3)$$

The two solutions of this polynom are the two *Eigenvalues* of the matrix:

$$\begin{aligned} \lambda_{1,2} &= \frac{1}{2} \left( a + d \pm \sqrt{(a + d)^2 - 4(ad - cb)} \right) \\ &= \frac{1}{2} \left( a + d \pm \sqrt{(a - d)^2 + 4cb} \right). \end{aligned} \quad (4)$$

Assuming all elements a,b,c,d to be real, then the Eigenvalues are real when the expression under the square-root is positiv  $(a - d)^2 + 4cb > 0$ , otherwise they are a complex conjugate pair.

The two vectors  $\mathbf{r}_i$ , ( $i=1,2$ ), which fulfill the Eigenvalue-equation for the two Eigenvalues  $\lambda_i$

$$\mathbf{H} \mathbf{r}_i = \lambda_i \mathbf{r}_i \quad (5)$$

are called the *Eigenvectors*. Thus, when the Eigenvalues have been calculated, one first inserts  $\lambda_1$  into eq.(2) and solves the resulting two linear equations for the two unkowns  $x_1$  and  $y_1$  of the first Eigenvector, subsequently the same is done to find the second Eigenvector. (For unsymmetrical matrices it may turn out, that two or more Eigenvectors collapse and become identical. See below: Defective Matrix).

Note that one of the two components of the Eigenvector can be freely determined, unless it is exactly zero.

Choosing for both Eigenvectors the first element  $x_i = 1$ , one obtains for the second element

$$y_i = \frac{\lambda_i - a}{b}. \quad (6)$$

When accidentally  $b = 0$ , then one can choose  $y_i = 1$  instead and  $x_i = 0$ .

Usually one normalizes the length of the Eigenvectors afterwards to the value 1.

In most cases - as we are assuming here also - the Eigenvectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are linearly independent or even orthogonal. If the Eigenvalues are complex, the Eigenvectors also are complex, but complex Eigenvectors do not imply complex Eigenvalues! The scalar product for complex vectors is defined as

$$\mathbf{r}_i^* \cdot \mathbf{r}_j \quad \text{scalar product for complex vectors} \quad (7)$$

### Example 1: Real Symmetric Matrix

$$\begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \quad (8)$$

$a = 1, b = 2, c = 2, d = 1$ . Eigenvalues in this case are  $\lambda_1 = 3$  und  $\lambda_2 = -1$ . Normalized Eigenvectors are

$$\mathbf{r}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathbf{r}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (9)$$

The Eigenvectors here are orthogonal:  $\mathbf{r}_1 \cdot \mathbf{r}_2 = 0$ !

### Example 2: Real Antisymmetric Matrix

$$\begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \quad (10)$$

$a = 1, b = 2, c = -2, d = 1$ . Eigenvalues form a complex conjugate pair:  $\lambda_1 = 1 + 2i$  und  $\lambda_2 = 1 - 2i$ . Eigenvectors are:

$$\mathbf{r}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad \mathbf{r}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \quad (11)$$

These Eigenvectors also are orthogonal to each other.

# Perturbation Theory

We assume now that we have an operator  $\mathbf{H}$  (for example: Hamilton operator of quantum mechanics) which consists of two parts:  $\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1$ , an 'easy' part  $\mathbf{H}_0$  and a 'difficult' part or the perturbation  $\mathbf{H}_1$ . To demonstrate the procedure of perturbation analysis we use the simplest examples of 2 by 2 matrices.

First example: **Non-Degenerate Case.**

$$H_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad H_1 = \begin{pmatrix} 0 & w \\ w & 0 \end{pmatrix} \quad (12)$$

The perturbation  $w$  is assumed to be small compared to 1. eigenvalues and Eigenvectors should be evaluated to leading order in  $w$ . Eigenvalues in this case are

$$\lambda_1 = +(1 + \frac{1}{2}w^2); \quad \lambda_2 = -(1 + \frac{1}{2}w^2) \quad (13)$$

Normalized Eigenvectors are

$$r_1 = \begin{pmatrix} 1 \\ w/2 \end{pmatrix}; \quad r_2 = \begin{pmatrix} -w/2 \\ 1 \end{pmatrix} \quad (14)$$

This means that the *Eigenvalues vary quadratically* as  $O(w^2)$  while the *Eigenvectors vary linearly* as  $O(w)$  with the perturbation  $w$ .

Second example: **Degenerate Case.**

$$H_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad H_1 = \begin{pmatrix} 0 & w \\ w & 0 \end{pmatrix} \quad (15)$$

Note that in this case of degenerate Eigenvalues, the two Eigenvectors of the unperturbed Hamiltonian  $\mathbf{H}_0$  are orthogonal to each other, but not fixed in absolute direction. This means that we can write

$$r_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad r_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (16)$$

but equally well could we write

$$r_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad r_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (17)$$

or other orthogonal expressions.

The perturbation  $w$  again is assumed to be small compared to 1. Eigenvalues and Eigenvectors should be evaluated to leading order in  $w$ . Eigenvalues in this case are

$$\lambda_1 = 1 + w; \quad \lambda_2 = 1 - w \quad (18)$$

Normalized Eigenvectors are now fixed as

$$r_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad r_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (19)$$

This means that the *Eigenvalues vary linearly* as  $O(w)$  while the *Eigenvectors* are to leading order independent of  $w$  but *fixed in direction* by an arbitrarily small perturbation  $w$ .

## Defective Matrix

An unsymmetrical matrix with collapsing Eigenvectors cannot be simply diagonalized. A small perturbation, however, may cure this to some extent. More generally, one must use *generalized eigenvectors* to form a complete set of vectors which span the whole space. - The respective theory of the *Jordan Normal Form* will not be considered further here.

As a simple example of this problem consider the non-symmetrical Matrix  $A = \begin{bmatrix} 0 & 1 \\ w & 0 \end{bmatrix}$  with two Eigenvalues, which are zero when the perturbation  $w$  is switched off:

$$\begin{pmatrix} 0 & 1 \\ w & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \quad (20)$$

The Eigenvalues are  $\lambda_{1,2} = \pm\sqrt{w}$ , the Eigenvectors are

$$r_{1,2} = \begin{pmatrix} 1 \\ \pm\sqrt{w} \end{pmatrix} \quad (21)$$

In this case, Eigenvalues and Eigenvectors vary with the same (fractional) power of the perturbation  $w$ , while for  $w=0$  only one Eigenvector survives!

# Symmetrical and Orthogonal Matrix

Symmetrical matrices are diagonalized by a similarity transform with an orthogonal matrix. We define the *symmetrical matrix*  $A = \begin{bmatrix} a & b \\ b & d \end{bmatrix}$

$$A = \begin{pmatrix} a & b \\ b & d \end{pmatrix} \quad (22)$$

We then define the *orthogonal matrix*  $R = \begin{bmatrix} \cos(\phi) & \sin(\phi) \\ -\sin(\phi) & \cos(\phi) \end{bmatrix}$

$$R = \begin{pmatrix} \cos(\phi) & \sin(\phi) \\ -\sin(\phi) & \cos(\phi) \end{pmatrix} \quad (23)$$

We also define the *invers orthogonal matrix*  $R^{-1}$

$$R^{-1} = \begin{pmatrix} \cos(\phi) & -\sin(\phi) \\ \sin(\phi) & \cos(\phi) \end{pmatrix} \quad (24)$$

As one can check easily, the column vectors of both orthogonal matrices are indeed orthogonal, as their scalar products vanish. Multiplying  $R * R^{-1} = R^{-1} * R = 1$  gives the unit matrix, for arbitrary angle  $\phi$ .

Now we try the following matrix *similarity transformation*:  $R^{-1} * A * R = \Lambda$ , hoping that  $\Lambda$  can be turned into a diagonal matrix by adjusting the angle  $\phi$  appropriately:

$$\begin{pmatrix} \cos & -\sin \\ \sin & \cos \end{pmatrix} * \begin{pmatrix} a & b \\ b & d \end{pmatrix} * \begin{pmatrix} \cos & \sin \\ -\sin & \cos \end{pmatrix} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \quad (25)$$

Performing the matrix multiplications, one arrives at the condition  $acs + bcc - bss - dcs = 0$ , where we have abbreviated 'c' for  $\cos(\phi)$ , and 's' for  $\sin(\phi)$ . The resulting condition for  $\phi$  then becomes

$$\left( \frac{\cos(\phi)}{\sin(\phi)} - \frac{\sin(\phi)}{\cos(\phi)} \right) = \frac{d - a}{b} \quad (26)$$

The Eigenvalues then are  $\lambda_1 = acc + dss - 2bcs$ ,  $\lambda_2 = ass + dcc + 2bcs$ . The columns of the orthogonal matrix  $R$  are the Eigenvectors. Compare this with the special cases discussed above.

# Diagonalization of Differential Equations

**Example a):** The following system of linear first order differential equations describes **rotation on a circle** around the origin of the x,y-plane. We define as usual  $\frac{d}{dt}x(t) = \dot{x}$ . The solution is obtained with the Ansatz

$$x_i(t) = \hat{x}_i \exp(\lambda_i t), \quad y_i(t) = \hat{y}_i \exp(\lambda_i t) \quad (27)$$

with Eigenvalues  $\lambda_1, \lambda_2$ , and amplitudes  $\hat{x}_i, \hat{y}_i$  for the initial values:

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad (28)$$

Eigenvalues are

$$\lambda_1 = +i; \quad \lambda_2 = -i \quad (29)$$

Eigenvectors are

$$r_1 = \begin{pmatrix} 1 \\ -i \end{pmatrix}; \quad r_2 = \begin{pmatrix} 1 \\ +i \end{pmatrix} \quad (30)$$

The general solution is now obtained by a linear combination of the two Eigenvectors, with arbitrary prefactors A and B:

$$r = A r_1 e^{\lambda_1 t} + B r_2 e^{\lambda_2 t} \quad (31)$$

(Note that  $r, r_1, r_2$  are two-component vectors).

Simplifying this to the special case A=B=1/2, we obtain

$$r(t) = \begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{it} + \frac{1}{2} \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-it} \quad (32)$$

which can be combined to give the final solution

$$r(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} e^{+it} + e^{-it} \\ -ie^{it} + ie^{-it} \end{pmatrix} = \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix} \quad (33)$$

**Example b): Hyperbolic motion** near the origin

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad (34)$$

Eigenvalues are

$$\lambda_1 = +1; \quad \lambda_2 = -1 \quad (35)$$

Eigenvectors are

$$r_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad r_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (36)$$

The general solution is obtained by a linear combination of the two Eigenvectors, with arbitrary prefactors A and B:

$$r = A r_1 e^{\lambda_1 t} + B r_2 e^{\lambda_2 t} \quad (37)$$

(Note that  $r, r_1, r_2$  are two-component vectors).

Simplifying this to the special case A=B=1, we obtain

$$r(t) = \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{+t} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-t} \quad (38)$$

which can be combined to give the final solution

$$r(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} e^{+t} \\ e^{-t} \end{pmatrix} \quad (39)$$

which obviously is a rather trivial case here.

**Example c): Spiraling rotation** around and towards the origin of the x,y-plane

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -w & -1 \\ 1 & -w \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad (40)$$

Eigenvalues are

$$\lambda_1 = -w + i; \quad \lambda_2 = -w - i \quad (41)$$

Eigenvectors are

$$r_1 = \begin{pmatrix} 1 \\ -i \end{pmatrix}; \quad r_2 = \begin{pmatrix} 1 \\ +i \end{pmatrix} \quad (42)$$

The general solution is obtained by a linear combination of the two Eigenvectors, with arbitrary prefactors A and B:

$$r = A r_1 e^{\lambda_1 t} + B r_2 e^{\lambda_2 t} \quad (43)$$

(Note that  $r, r_1, r_2$  are two-component vectors).

Simplifying this to the special case A=B=1/2, we obtain



$$r(t) = \begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-wt+it} + \frac{1}{2} \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-wt-it} \quad (44)$$

which can be combined to give the final solution

$$r(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \frac{1}{2} e^{-wt} \begin{pmatrix} e^{+it} + e^{-it} \\ -ie^{it} + ie^{-it} \end{pmatrix} = e^{-wt} \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix} \quad (45)$$

This is a spiral going around the origin,  $w$  being the rate of convergence towards the origin.

## Hermitian and Unitary Matrix

In quantum mechanics, because of the complex nature of the wavefunction, we usually do not have symmetrical matrices but Hermite (or Hermitian) matrices. They are also called self-adjoint. A Hermite matrix  $H = [a, b + i\beta]; [b - i\beta, d]$  with  $a, b, \beta, d =$  all real, looks like

$$\begin{pmatrix} a & b + i\beta \\ b - i\beta & d \end{pmatrix} \quad (46)$$

*A Hermitian matrix has real Eigenvalues!* A Hermitian matrix  $H$  is diagonalized by a similarity transform with a *unitary matrix*  $U$ .

### Properties of important matrices:

$A$  : square matrix

$A^T$  : transposed matrix (rows and columns interchanged)

$A^T = A$  : symmetrical matrix

$A^{-1}$  : inverse matrix,  $A^{-1} * A = A * A^{-1} = 1$

$A^T = A^{-1}$  : orthogonal matrix

$A^*$  : complex conjugate matrix (signs of imaginary parts inverted)

$A^+$  : adjoint matrix (rows and columns interchanged, and signs of imaginary parts inverted)

$A^+ = A$  : Hermitian matrix !

$A^+ = A^{-1}$  : unitary matrix

The Hermitian matrix  $H$  is diagonalized with a unitary matrix  $U$  by the similarity transform  $U^+ * H * U = \Lambda$ , and the Eigenvalues are real!

Performing one of the operations  $X^T, X^+, X^{-1}$  on matrix products  $X=AB$ , one interchanges the matrices and then performs the operation:  $(AB)^+ = (B^+ A^+)$ . Analogously for the other operations.