



Laboratory Techniques and Medical Device Approvals I

Part 03: Basics in Matrix Calculations



Mathematical basics

Basics in statistics and matrix calculations
relevant for the Principle Component Analysis



- Average / Mean: $\bar{X} = \frac{\sum_{i=1}^n X_i}{n}$
 - Standard deviation: $sdv(X) = \sqrt{\frac{\sum_{i=1}^n (X_i - \bar{X})^2}{(n-1)}}$
 - Variance: $var(X) = sdv^2(X) = \frac{\sum_{i=1}^n (X_i - \bar{X})^2}{(n-1)}$
 - Covariance: $cov(X, Y) = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$
- note: $var(X) = cov(X, X)$



- Matrix notation:

$$A_{(m,n)} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ a_{m2} & \dots & \dots & a_{mn} \end{bmatrix}$$

(m,n) are the matrix dimensions

- A vector $\vec{v} = \begin{pmatrix} a_1 \\ a_2 \\ \dots \\ a_m \end{pmatrix}$ can be regarded as a (m,1)-Matrix



- The main diagonal of a matrix is the collection of entries $A_{i,j}$ where i is equal to j :

$$A_{(3,2)} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}$$

- A square matrix in which the entries outside the main diagonal are all zero is called a **diagonal matrix**.
- A diagonal matrix with ones on the main diagonal is called an **identity matrix (I)**.

$$I_1 = (1) \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{etc.}$$



- **Matrix addition:**

- Works only with matrices of the same dimensions
- The elements of a matrix are added together with the corresponding elements of the second matrix.

$$A_{(m,n)} + B_{(m,n)} = (a_{ij} + b_{ij})$$

- Example:

$$\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} + \begin{bmatrix} 4 & 3 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 1+4 & 3+3 \\ 2+2 & 4+1 \end{bmatrix} = \begin{bmatrix} 5 & 6 \\ 4 & 5 \end{bmatrix}$$



- **Matrix multiplication** with a scalar k :

$$k \cdot A = A \cdot k = k \cdot \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ a_{m2} & \dots & \dots & a_{mn} \end{bmatrix}$$

$$= \begin{bmatrix} k \cdot a_{11} & k \cdot a_{12} & \dots & k \cdot a_{1n} \\ k \cdot a_{21} & k \cdot a_{22} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ k \cdot a_{m2} & \dots & \dots & k \cdot a_{mn} \end{bmatrix}$$



- **Matrix multiplication of two matrices:**

- **Not** commutative: $A \cdot B \neq B \cdot A$
- Number of columns of the first matrix has to be equal to the number of rows of the second matrix.

- For $A_{(l,m)} = (a_{ij})$ and $B_{(m,n)} = (b_{ij})$ is $A_{(l,m)} \cdot B_{(m,n)} = C_{(l,n)}$

with
$$c_{ij} = \sum_{k=1}^m a_{ik} \cdot b_{kj}$$

- The dimension of the matrix product is predefined by the two factor matrices. The number of rows is determined by the first factor matrix and the number of columns by the second factor matrix.



- **Manual matrix multiplication:**
 - Can be performed with the help of the **Falk's Scheme**
 - Both factor matrices are written in **parallel** with a **height offset**.
 - The **row elements** of the **first factor matrix** are multiplied with the corresponding **column elements** of the **second factor matrix**.
 - The results of each row are summed up and written into the appropriate position of the matrix product (intersection of the corresponding rows and columns).



Matrix multiplication

- Example:

$$A_{(3,2)} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & -6 \end{bmatrix} \quad B_{(2,2)} = \begin{bmatrix} -1 & 1 \\ 1 & -2 \end{bmatrix}$$

Diagram illustrating the calculation of the third row of the product matrix $A \cdot B$. Arrows show the dot product of the third row of A with the first and second columns of B .

$$\begin{bmatrix} 3 & -7 \\ 3 & -8 \\ -9 & 15 \end{bmatrix} \quad 1 \cdot (-1) + (4 \cdot 1) = 3$$



- **Special case: Multiplication of a matrix with a vector**
 - The matrix must have as many columns as the vector elements
 - The product of a **(m,n) -matrix** with a **n -dimensional vector** results in a **vector with the dimension m** .

Example:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \cdot \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} (1 \cdot 1 + 2 \cdot 2 + 3 \cdot 3) \\ (4 \cdot 1 + 5 \cdot 2 + 6 \cdot 3) \end{pmatrix} = \begin{pmatrix} 14 \\ 32 \end{pmatrix}$$



Transpose of a matrix

- **Transpose of a matrix:**

- „Reflection“ at the main diagonal or exchange of rows and columns

$$A_{(3,2)} = \begin{bmatrix} 1 & 6 \\ 2 & 5 \\ 3 & 4 \end{bmatrix}$$

$$A^T = \begin{bmatrix} 1 & 2 & 3 \\ 6 & 5 & 4 \end{bmatrix}$$

Calculation rules: $(A + B)^T = A^T + B^T$

$$(c \cdot A)^T = c \cdot A^T$$

$$(A^T)^T = A$$

$$(A \cdot B)^T = B^T \cdot A^T$$

$$(A^{-1})^T = (A^T)^{-1}$$

A square matrix whose transpose is equal to itself is called a **symmetric matrix**.

$$A = A^T$$



- **Inverse matrix:**

- If the following equation is valid for the matrices A and B,

$$A \cdot B = B \cdot A = I$$

I = Identity matrix

then B is the inverse matrix of A: $B = A^{-1}$



- **Methods of matrix inversion**

- Gauss-Jordan-Algorithm:
- Algorithm for solving **systems of linear equations**
- The identity matrix is augmented to the right of the matrix A forming a n by $2n$ **block matrix** $\left[A \mid I \right]$
- Through application of elementary row operations to both matrices the matrix A is reduced to the identity matrix I .
- The matrix A is invertible if it can be reduced to the identity matrix I . In this case the former identity matrix is the inverse matrix A^{-1} .



• Example: $A = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 3 & 0 \\ 3 & 4 & 1 \end{bmatrix}$

- Write as a block matrix $\left[A \mid I \right]$ and solve the system of linear equations:

$$\begin{array}{l} I \\ II \\ III \end{array} \left[\begin{array}{ccc|ccc} 1 & 2 & 0 & 1 & 0 & 0 \\ 2 & 3 & 0 & 0 & 1 & 0 \\ 3 & 4 & 1 & 0 & 0 & 1 \end{array} \right] \begin{array}{l} \\ -(2 \cdot I) \\ -(3 \cdot I) \end{array}$$



$$\begin{array}{l} I \\ II \\ III \end{array} \left[\begin{array}{ccc|ccc} 1 & 2 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & -2 & 1 & 0 \\ 0 & -2 & 1 & -3 & 0 & 1 \end{array} \right] \begin{array}{l} +(2 \cdot II) \\ \cdot(-1) \\ -(2 \cdot II) \end{array}$$

$$\begin{array}{l} I \\ II \\ III \end{array} \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -3 & 2 & 0 \\ 0 & 1 & 0 & 2 & -1 & 0 \\ 0 & 0 & 1 & 1 & -2 & 1 \end{array} \right]$$



• The inverse of $A = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 3 & 0 \\ 3 & 4 & 1 \end{bmatrix}$

is $A^{-1} = \begin{bmatrix} -3 & 2 & 0 \\ 2 & -1 & 0 \\ 1 & -2 & 1 \end{bmatrix}$

Crosscheck:

Multiply the matrix by its inverse matrix. You should get the identity matrix.

$$A \cdot A^{-1} = I$$



- **Determinant of a matrix:**

- Exists only for square matrices
- Is good for the calculation of eigenvectors
- Provides information about the possibility of matrix inversion
(the system of linear equations has a unique solution when the determinant is nonzero)



Determination of the determinant:

- E. g.: **Gaussian elimination:**
 - Works for the special case of an **upper triangular matrix**: The determinant is the **product of the main diagonal elements**.
 - With the Gaussian elimination square matrices can be transferred into upper triangular matrices



- Transformation rules for the Gaussian elimination:
 - If two rows or columns of a matrix are **exchanged**, then **changes the sign** of the determinant.
 - If a multiple of a row or column is **added to another** row or column, then the determinant **does not change**
 - If a row or column is **multiplied** by a factor, then the resulting determinant has to be **divided** by this factor.



- Example: Transformation of a matrix into a triangular matrix

$$A_{(4,4)} = \begin{bmatrix} 1 & 2 & 4 & 1 \\ -1 & 3 & 2 & 0 \\ 2 & 0 & 0 & -2 \\ 2 & 3 & 2 & -1 \end{bmatrix} \begin{matrix} I \\ II \\ III \\ IV \end{matrix}$$

$\begin{matrix} a & b & c & d \end{matrix}$

- **Step 1:** exchange a and d (**change of sign!**)



Determinant of a matrix

$$A_{(4,4)} = \begin{bmatrix} 1 & 2 & 4 & 1 \\ 0 & 3 & 2 & -1 \\ -2 & 0 & 0 & 2 \\ -1 & 3 & 2 & 2 \\ a & b & c & d \end{bmatrix} \begin{matrix} I \\ II \\ III \\ IV \end{matrix}$$

- **Step 2:** Add 2 times row *I* to row *III* and one time row *I* to row *IV*

$$A_{(4,4)} = \begin{bmatrix} 1 & 2 & 4 & 1 \\ 0 & 3 & 2 & -1 \\ 0 & 4 & 8 & 4 \\ 0 & 5 & 6 & 3 \end{bmatrix} \begin{matrix} I \\ II \\ III \\ IV \end{matrix}$$

- **Step 3:** Subtract 0.5 times column *c* from column *b*



Determinant of a matrix

$$A_{(4,4)} = \begin{bmatrix} 1 & 0 & 4 & 1 \\ 0 & 2 & 2 & -1 \\ 0 & 0 & 8 & 4 \\ 0 & 2 & 6 & 3 \\ a & b & c & d \end{bmatrix} \begin{matrix} I \\ II \\ III \\ IV \end{matrix}$$

- **Step 4:** Subtract row *II* from row *IV*

$$A_{(4,4)} = \begin{bmatrix} 1 & 0 & 4 & 1 \\ 0 & 2 & 2 & -1 \\ 0 & 0 & 8 & 4 \\ 0 & 0 & 4 & 4 \end{bmatrix} \begin{matrix} I \\ II \\ III \\ IV \end{matrix}$$

- **Step 5:** Subtract 0.5 times row *III* from row *IV*



Determinant of a matrix

$$A_{(4,4)} = \begin{bmatrix} 1 & 0 & 4 & 1 \\ 0 & 2 & 2 & -1 \\ 0 & 0 & 8 & 4 \\ 0 & 0 & 0 & 2 \end{bmatrix} \begin{matrix} I \\ II \\ III \\ IV \end{matrix}$$

$a \quad b \quad c \quad d$

$$\det(A) = 1 \cdot 2 \cdot 8 \cdot 2 \cdot (-1) = -32$$

↑
Change of sign

- **Step 6:** Calculate the product of the main diagonal elements of this upper triangular matrix
- **Step 7:** Change sign if you had an odd number of exchange operations, otherwise keep it. (**here:** only one exchange operation in step 1 => change sign)



- **Eigenvectors of a matrix:**

- If you multiply a square (n,n)- matrix with a n-dimensional vector, then this vector is transformed.
- If the transformed vector is a scalar multiple of the initial vector (change in length, but not in orientation), then it is an **eigenvector** of the square (n,n)- matrix.
- The scale factor is the **eigenvalue** of the corresponding eigenvector.
- A (n,n)-matrix has n linear independent eigenvectors
- Eigenvectors and eigenvalues can be computed by solving the system of linear equations $(A - \lambda I)\vec{x} = \vec{0}$ with $\vec{x}$ = Eigenvector and λ = Eigenvalue.

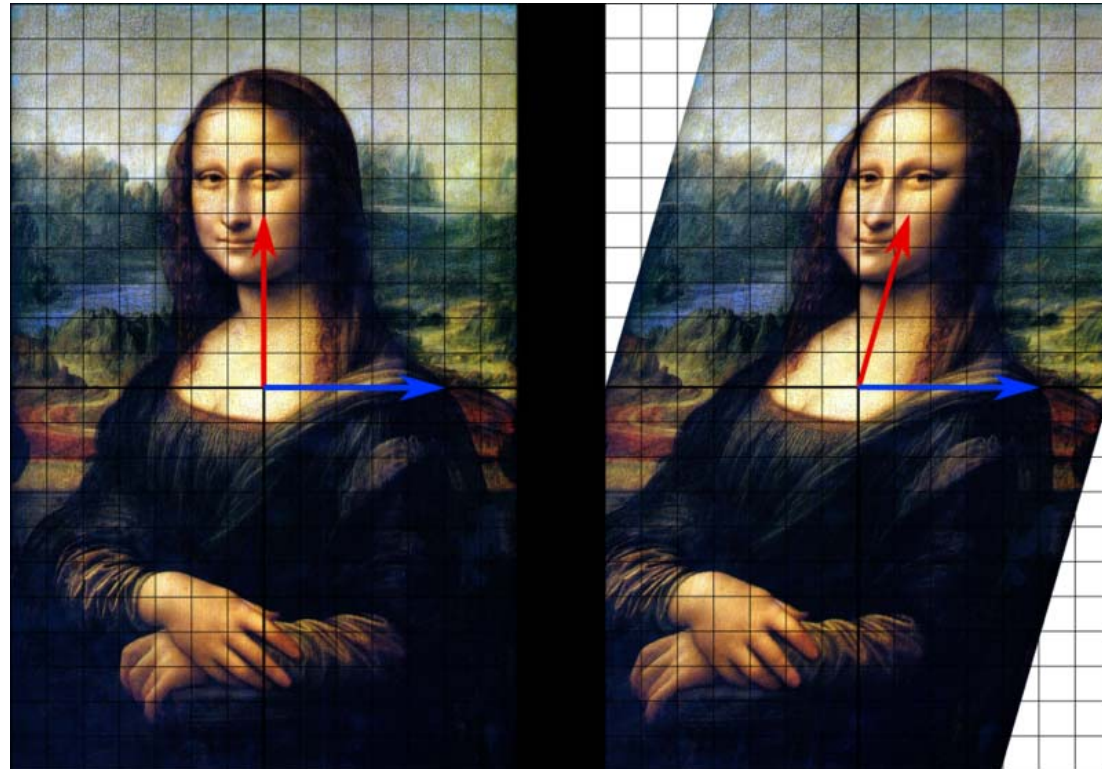


Eigenvectors /Eigenvalues of a matrix

Shear mapping of the Mona Lisa.

The blue vector stays unchanged, whereas the red one changes upon shear.

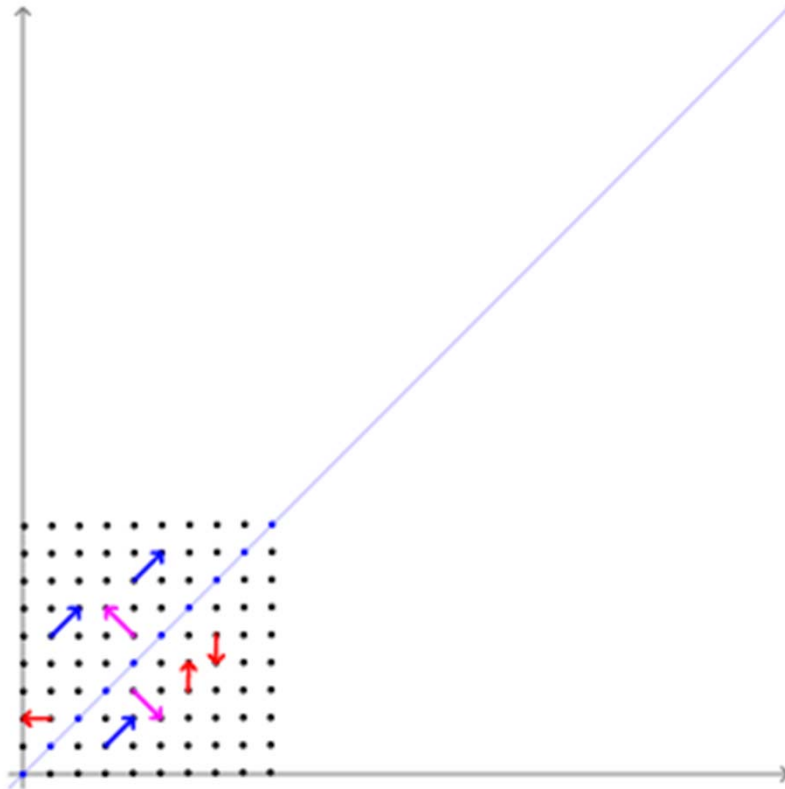
⇒ The blue vector is an eigenvector



Source: Wikipedia



Eigenvectors /Eigenvalues of a matrix



The transformation matrix
 $\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$ preserves the
 direction of vectors parallel
 to $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$.
 $\Rightarrow$ Eigenvectors

The vectors in red are not
 eigenvectors, therefore their
 direction is altered by the
 transformation.



Eigenvectors /Eigenvalues of a matrix

- The system of linear equations can be computed, if

$$\det(A - \lambda I) = 0$$

- The eigenvalues of a matrix can be determined by finding the roots of the characteristic polynomial. $\chi_A(\lambda)$

$$\chi_A(\lambda) = \det(\lambda I - A)$$

- **A (n,n)-Matrix has a characteristic polynomial with degree n**
- n-dimensional matrices can be solved by iterative algorithms, e.g. SVD (**S**ingular **V**alue **D**ecomposition) or NIPALS (**N**onlinear **I**terative **P**artial **L**east **S**quares).



Eigenvectors /Eigenvalues of a matrix

Example: Calculate the eigenvalues and eigenvectors of (2,2)-Matrix (characteristic polynomial with degree 2)

$$A_{(2,2)} = \begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix} \quad \lambda I - A = \begin{bmatrix} \lambda - 2 & -3 \\ -2 & \lambda - 1 \end{bmatrix}$$

Note: The determinant for a (2,2)-matrix is

$$\det(A) = a_{11} \cdot a_{22} - a_{12} \cdot a_{21}$$

here $\det(\lambda I - A) = (\lambda - 2) \cdot (\lambda - 1) - (-3) \cdot (-2)$

$$\Rightarrow \chi_A(\lambda) = \det(\lambda I - A) = \lambda^2 - 3\lambda - 4$$



Eigenvectors /Eigenvalues of a matrix

- The eigenvalues of the matrix A can be computed by solving the following equation:

$$\lambda^2 - 3\lambda - 4 = 0$$

$$\lambda_{1,2} = \frac{3 \pm \sqrt{(-3)^2 - 4 \cdot 1 \cdot (-4)}}{2}$$

$$\left. \begin{array}{l} \lambda_1 = 4 \\ \lambda_2 = -1 \end{array} \right\} \text{Eigenvalues of } A$$



Eigenvectors /Eigenvalues of a matrix

- Put the eigenvalues into the system of linear equations

$$(A - \lambda I)\vec{x} = 0$$

and calculate the eigenvectors $\vec{x}$ and $\vec{y}$ of the matrix

$$\text{Eigenvector } \vec{x} : \begin{bmatrix} 2-4 & 3 \\ 2 & 1-4 \end{bmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \stackrel{!}{=} 0$$

Then one has

$$-2x_1 + 3x_2 = 0 \quad \Leftrightarrow \quad x_1 = 1,5x_2$$

$$2x_1 - 3x_2 = 0$$

$$\vec{x} = \begin{pmatrix} 1 \\ 1,5 \end{pmatrix}$$

and consequently the eigenvector $\vec{x}$ is



Eigenvectors /Eigenvalues of a matrix

- The modulus of the eigenvector has no significance. Therefore, it can be normalized to the length 1:

$$\sqrt{(x_1)^2 + (x_2)^2} = 1$$

- With:

$$x_1 = 1,5 \cdot x_2$$

$$\hookrightarrow \sqrt{(1,5 \cdot x_2)^2 + (x_2)^2} = \sqrt{3,25x_2^2} = 1$$

$$\Leftrightarrow 1,8x_2 = 1 \Leftrightarrow x_2 = 0,55$$



Eigenvectors /Eigenvalues of a matrix

- Put x_2 into the system of linear equations. Then one obtains for x_1 :

$$2x_1 - 3 \cdot 0,55 = 0 \Leftrightarrow 1,5 \cdot 0,55 = x_1$$

$$x_1 = 0,825$$

- The normalized eigenvector of $\vec{x}$ is $\vec{x} = \begin{pmatrix} 0,825 \\ 0,55 \end{pmatrix}$

- The same procedure with the second eigenvalue $\lambda_2 = -1$ results in the second normalized eigenvector

$$\vec{y} = \begin{pmatrix} -1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{2}} \quad \text{auf 1 skalieren!}$$



Examination relevant results

- Mathematical basis
- Performing of
 - Simple matrix operations (sum, difference, etc.)
 - Matrix multiplication
 - Matrix inversion
 - Calculation of a determinant
- Verbal explanation of an Eigenvector



END of Part 03