A. A REMINDER: MATRICES AND DETERMINANTS

1 MATRICES

Definition

A $n \times m$ matrix $\boldsymbol{A}$ represents a rectangular table of numbers[1] A_{ij} standing like soldiers in n perfect rows and m columns (index i tells us in which row, and index j tells in which column the number A_{ij} is located)

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ \dots & \dots & \dots & \dots \\ A_{n1} & A_{n2} & \dots & A_{nm} \end{pmatrix}.$$

Such a notation allows us to operate whole matrices (like troops), instead of specifying what happens to each number ("soldier") separately. If matrices were not invented, the equations would be very long and clumsy, instead they are short and clear.

Addition

Two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ may be *added* if their dimensions n and m match. The result is matrix $\boldsymbol{C} = \boldsymbol{A} + \boldsymbol{B}$ (of the same dimensions as $\boldsymbol{A}$ and $\boldsymbol{B}$), where each element of $\boldsymbol{C}$ is the sum of the corresponding elements of $\boldsymbol{A}$ and $\boldsymbol{B}$:

$$C_{ij} = A_{ij} + B_{ij},$$

e.g.,

$$\begin{pmatrix} 1 & -1 \\ -3 & 4 \end{pmatrix} + \begin{pmatrix} 2 & 1 \\ -2 & 3 \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ -5 & 7 \end{pmatrix}.$$

Multiplying by a number

A matrix may be multiplied by a number by multiplying every element of the matrix by this number: $c\boldsymbol{A} = \boldsymbol{B}$ with $B_{ij} = cA_{ij}$. For example, $2\begin{pmatrix} 1 & -1 \\ 3 & -2 \end{pmatrix} = \begin{pmatrix} 2 & -2 \\ 6 & -4 \end{pmatrix}$.

[1] If instead of numbers a matrix contained functions, everything below would remain valid (at particular values of the variables instead of functions we would have their values).

Matrix product

The product of two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ is matrix $\boldsymbol{C}$ denoted by $\boldsymbol{C}=\boldsymbol{A}\boldsymbol{B}$, its elements are calculated using elements of $\boldsymbol{A}$ and $\boldsymbol{B}$:

$$C_{ij}=\sum_{k=1}^{N} A_{ik}B_{kj},$$

where the number of columns (N) of matrix $\boldsymbol{A}$ has to be equal to the number of rows of matrix $\boldsymbol{B}$. The resulting matrix $\boldsymbol{C}$ has the number of rows equal to the number of rows of $\boldsymbol{A}$ and the number of columns equal to the number of columns of $\boldsymbol{B}$. Let us see how it works in an example. The product $\boldsymbol{A}\boldsymbol{B}=\boldsymbol{C}$:

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ \boldsymbol{A_{21}} & \boldsymbol{A_{22}} & \boldsymbol{A_{23}} & \boldsymbol{A_{24}} \\ A_{31} & A_{32} & A_{33} & A_{34} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & \boldsymbol{B_{13}} & B_{14} & B_{15} & B_{16} & B_{17} \\ B_{21} & B_{22} & \boldsymbol{B_{23}} & B_{24} & B_{25} & B_{26} & B_{27} \\ B_{31} & B_{32} & \boldsymbol{B_{33}} & B_{34} & B_{35} & B_{36} & B_{37} \\ B_{41} & B_{42} & \boldsymbol{B_{43}} & B_{44} & B_{45} & B_{46} & B_{47} \end{pmatrix}$$
$$= \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} & C_{17} \\ C_{21} & C_{22} & \boldsymbol{C_{23}} & C_{24} & C_{25} & C_{26} & C_{27} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} & C_{37} \end{pmatrix},$$

e.g., C_{23} is simply the dot product of two vectors or in matrix notation

$$C_{23} = \begin{pmatrix} A_{21} & A_{22} & A_{23} & A_{24} \end{pmatrix} \cdot \begin{pmatrix} B_{13} \\ B_{23} \\ B_{33} \\ B_{43} \end{pmatrix}$$
$$= A_{21}B_{13} + A_{22}B_{23} + A_{23}B_{33} + A_{24}B_{43}.$$

Some remarks:

- The result of matrix multiplication depends in general on whether we have to multiply $\boldsymbol{A}\boldsymbol{B}$ or $\boldsymbol{B}\boldsymbol{A}$, i.e. $\boldsymbol{A}\boldsymbol{B}\neq\boldsymbol{B}\boldsymbol{A}$.[2]
- Matrix multiplication satisfies the relation (easy to check): $\boldsymbol{A}(\boldsymbol{B}\boldsymbol{C})=(\boldsymbol{A}\boldsymbol{B})\boldsymbol{C}$, i.e. the parentheses do not count and we can simply write: $\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}$.
- Often we will have multiplication of a square matrix $\boldsymbol{A}$ by a matrix $\boldsymbol{B}$ composed of one column. Then, using the rule of matrix multiplication, we obtain matrix $\boldsymbol{C}$ in the form of a single column (with the number of elements identical to the dimension of $\boldsymbol{A}$):

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ \dots & \dots & \dots & \dots \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \\ \dots \\ B_m \end{pmatrix} = \begin{pmatrix} C_1 \\ C_2 \\ \dots \\ C_m \end{pmatrix}.$$

[2]Although it may happen, that $\boldsymbol{A}\boldsymbol{B}=\boldsymbol{B}\boldsymbol{A}$.

Transposed matrix

For a given matrix $\boldsymbol{A}$ we may define the transposed matrix $\boldsymbol{A}^T$ defined as $(\boldsymbol{A}^T)_{ij} = \boldsymbol{A}_{ji}$.

For example,

$$\text{if } \boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ -2 & 3 \end{pmatrix}, \text{ then } \boldsymbol{A}^T = \begin{pmatrix} 1 & -2 \\ 2 & 3 \end{pmatrix}.$$

If matrix $\boldsymbol{A} = \boldsymbol{BC}$, then $\boldsymbol{A}^T = \boldsymbol{C}^T\boldsymbol{B}^T$, i.e. the order of multiplication is reversed. Indeed, $(\boldsymbol{C}^T\boldsymbol{B}^T)_{ij} = \sum_k (\boldsymbol{C}^T)_{ik} (\boldsymbol{B}^T)_{kj} = \sum_k \boldsymbol{C}_{ki} \boldsymbol{B}_{jk} = \sum_k \boldsymbol{B}_{jk}\boldsymbol{C}_{ki} = (\boldsymbol{BC})_{ji} = (\boldsymbol{A}^T)_{ij}$.

Inverse matrix

For some square matrices $\boldsymbol{A}$ (which will be called non-singular) we can define what is called the inverse matrix denoted as $\boldsymbol{A}^{-1}$, which has the following property: $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \mathbf{1}$, where $\mathbf{1}$ stands for the unit matrix:

$$\mathbf{1} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \end{pmatrix}.$$

For example, for matrix $\boldsymbol{A} = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$ we can find $\boldsymbol{A}^{-1} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{pmatrix}$.

For square matrices $\boldsymbol{A}\mathbf{1} = \mathbf{1}\boldsymbol{A} = \boldsymbol{A}$.

If we cannot find $\boldsymbol{A}^{-1}$ (because it does not exist), $\boldsymbol{A}$ is called a singular matrix. singular matrix

For example, matrix $\boldsymbol{A} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ is singular. The inverse matrix for $\boldsymbol{A} = \boldsymbol{BC}$ is $\boldsymbol{A}^{-1} = \boldsymbol{C}^{-1}\boldsymbol{B}^{-1}$. Indeed, $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{BC}\boldsymbol{C}^{-1}\boldsymbol{B}^{-1} = \boldsymbol{B}\mathbf{1}\boldsymbol{B}^{-1} = \boldsymbol{B}\boldsymbol{B}^{-1} = \mathbf{1}$.

Adjoint, Hermitian, symmetric matrices

If matrix $\boldsymbol{A}$ is transposed and in addition all its elements are changed to their complex conjugate, we obtain the *adjoint matrix* denoted as $\boldsymbol{A}^\dagger = (\boldsymbol{A}^T)^* = (\boldsymbol{A}^*)^T$. If, for a square matrix, we have $\boldsymbol{A}^\dagger = \boldsymbol{A}$, $\boldsymbol{A}$ is called *Hermitian*. If $\boldsymbol{A}$ is real, then, of course, $\boldsymbol{A}^\dagger = \boldsymbol{A}^T$. If, in addition, for a real square matrix $\boldsymbol{A}^T = \boldsymbol{A}$, then $\boldsymbol{A}$ is called *symmetric*. Examples:

$$\boldsymbol{A} = \begin{pmatrix} 1+i & 3-2i \\ 2+i & 3-i \end{pmatrix};\ \boldsymbol{A}^T = \begin{pmatrix} 1+i & 2+i \\ 3-2i & 3-i \end{pmatrix};\ \boldsymbol{A}^\dagger = \begin{pmatrix} 1-i & 2-i \\ 3+2i & 3+i \end{pmatrix}.$$

Matrix $\boldsymbol{A} = \begin{pmatrix} 1 & -i \\ i & -2 \end{pmatrix}$ is an example of a Hermitian matrix, because $\boldsymbol{A}^\dagger = \boldsymbol{A}$. Matrix $\boldsymbol{A} = \begin{pmatrix} 1 & -5 \\ -5 & -2 \end{pmatrix}$ is a symmetric matrix.

Unitary and orthogonal matrices

If for a square matrix $\boldsymbol{A}$ we have $\boldsymbol{A}^\dagger = \boldsymbol{A}^{-1}$, $\boldsymbol{A}$ is called a *unitary* matrix. If $\boldsymbol{B}$ is Hermitian, the matrix $\exp(i\boldsymbol{B})$ is unitary, where we define $\exp(i\boldsymbol{B})$ by using the Taylor expansion: $\exp(i\boldsymbol{B}) = \mathbf{1} + i\boldsymbol{B} + \frac{1}{2!}(i\boldsymbol{B})^2 + \cdots$. Indeed, $[\exp(i\boldsymbol{B})]^\dagger = \mathbf{1} - i\boldsymbol{B}^T + \frac{1}{2!}(-i\boldsymbol{B}^T)^2 + \cdots = \mathbf{1} - i\boldsymbol{B} + \frac{1}{2!}(-i\boldsymbol{B})^2 + \cdots = \exp(-i\boldsymbol{B})$, while $\exp(i\boldsymbol{B})\exp(-i\boldsymbol{B}) = \mathbf{1}$.

If $\boldsymbol{A}$ is a real unitary matrix $\boldsymbol{A}^\dagger = \boldsymbol{A}^T$, it is called *orthogonal* with the property $\boldsymbol{A}^T = \boldsymbol{A}^{-1}$. For example, if

$$\boldsymbol{A} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \text{ then } \boldsymbol{A}^T = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \boldsymbol{A}^{-1}.$$

Indeed,

$$\boldsymbol{A}\boldsymbol{A}^T = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

2 DETERMINANTS

Definition

For any square matrix $\boldsymbol{A} = \{A_{ij}\}$ we may calculate a number called its determinant and denoted by $\det\boldsymbol{A}$ or $|\boldsymbol{A}|$. The determinant is calculated by using the Laplace expansion

$$\det\boldsymbol{A} = \sum_i^N (-1)^{i+j} A_{ij}\bar{A}_{ij} = \sum_j^N (-1)^{i+j} A_{ij}\bar{A}_{ij},$$

where (N is the dimension of the matrix) the result does not depend on which column j has been chosen in the first expression or which row i in the second expression. The symbol $\bar{A}_{ij}$ stands for the determinant of the matrix, which is obtained from $\boldsymbol{A}$ by removing the i-th row and the j-th column. Thus we have defined a determinant (of dimension N) by saying that it is a certain linear combination of determinants (of dimension $N-1$). It is then sufficient to say what we mean by a determinant that contains only one number c (i.e. has only one row and one column), this is simply $\det c \equiv c$.

For example, for matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & 0 & -1 \\ 2 & 2 & 4 \\ 3 & -2 & -3 \end{pmatrix},$$

its determinant is

$$\det\boldsymbol{A} = \begin{vmatrix} 1 & 0 & -1 \\ 2 & 2 & 4 \\ 3 & -2 & -3 \end{vmatrix} = (-1)^{1+1} \times 1 \times \begin{vmatrix} 2 & 4 \\ -2 & -3 \end{vmatrix} + (-1)^{1+2} \times 0 \times \begin{vmatrix} 2 & 4 \\ 3 & -3 \end{vmatrix}$$
$$+ (-1)^{1+3} \times (-1) \times \begin{vmatrix} 2 & 2 \\ 3 & -2 \end{vmatrix} = \begin{vmatrix} 2 & 4 \\ -2 & -3 \end{vmatrix} - \begin{vmatrix} 2 & 2 \\ 3 & -2 \end{vmatrix}$$

$$= \big(2 \times (-3) - 4 \times (-2)\big) - \big(2 \times (-2) - 2 \times 3\big)$$
$$= 2 + 10 = 12.$$

In particular, $\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc.$

By repeating the Laplace expansion again and again (i.e. expanding $\bar{A}_{ij}$, etc.) we finally arrive at a linear combination of the products of the elements

$$\det \boldsymbol{A} = \sum_P (-1)^p \hat{P}[A_{1\mathbf{1}} A_{2\mathbf{2}} \cdots A_{N\boldsymbol{N}}],$$

where the permutation operator $\hat{P}$ pertains to the second indices (shown in bold), and p is the parity of permutation $\hat{P}$.

Slater determinant

In this book we will most often have to do with determinants of matrices whose elements are functions, not numbers. In particular what are called Slater determinants will be the most important. A Slater determinant for the N -electron system is built of functions called spinorbitals $\phi_i(j)$, $i = 1, 2, \ldots, N$, where the *symbol* j denotes the space and spin coordinates $(x_j, y_j, z_j, \sigma_j)$ of electron j:

$$\psi(1, 2, \ldots, N) = \begin{vmatrix} \phi_1(1) & \phi_1(2) & \ldots & \phi_1(N) \\ \phi_2(1) & \phi_2(2) & \ldots & \phi_2(N) \\ \ldots & \ldots & \ldots & \ldots \\ \phi_N(1) & \phi_N(2) & \ldots & \phi_N(N) \end{vmatrix}.$$

After this is done the Laplace expansion gives

$$\psi(1, 2, \ldots, N) = \sum_P (-1)^p \hat{P}\big[\phi_1(1)\phi_2(2)\ldots\phi_N(N)\big],$$

where the summation is over $N!$ permutations of the N electrons, $\hat{P}$ stands for the permutation operator that acts on the *arguments* of the product of the spinorbitals $[\phi_1(1)\phi_2(2)\ldots\phi_N(N)]$, p is the parity of permutation $\hat{P}$ (i.e. the number of the transpositions that change $[\phi_1(1)\phi_2(2)\ldots\phi_N(N)]$ into $\hat{P}[\phi_1(1)\phi_2(2)\ldots\phi_N(N)]$.

All properties of determinants pertain also to Slater determinants.

Some useful properties

- $\det \boldsymbol{A}^T = \det \boldsymbol{A}$.
- From the Laplace expansion it follows that if one of the spinorbitals is composed of two functions $\phi_i = \xi + \zeta$, the Slater determinant is the sum of the two Slater determinants, one with ξ instead of ϕ_i, the second with ζ instead of ϕ_i.
- If we add to a row (column) any linear combination of other rows (columns), the value of the determinant does not change.

- If a row (column) is a linear combination of other rows (columns), then $\det \boldsymbol{A} = 0$. In particular, if two rows (columns) are identical then $\det \boldsymbol{A} = 0$. Conclusion: in a Slater determinant the spinorbitals have to be linearly independent, otherwise the Slater determinant is equal zero.
- If in a matrix $\boldsymbol{A}$ we exchange two rows (columns), then $\det \boldsymbol{A}$ changes sign. Conclusion: the exchange of the coordinates of any two electrons leads to a change of sign of the Slater determinant (Pauli exclusion principle).
- $\det(\boldsymbol{AB}) = \det \boldsymbol{A} \det \boldsymbol{B}$.
- From the Laplace expansion it follows that multiplying the determinant by a number is equivalent to multiplication of an arbitrary row (column) by this number. Therefore, $\det(c\boldsymbol{A}) = c^N \det \boldsymbol{A}$, where N is the matrix dimension.[3]
- If matrix $\boldsymbol{U}$ is unitary then $\det \boldsymbol{U} = \exp(i\phi)$, where ϕ is a real number. This means that if $\boldsymbol{U}$ is an orthogonal matrix, $\det \boldsymbol{U} = \pm 1$.

[3]Note, that to multiply a matrix by a number we have to multiply every element of the matrix by this number. However, to multiply a determinant by a number means multiplication of one row (column) by this number.