Vectors as a list of associated information

\[ \vec{x} = \begin{pmatrix} \text{number of steps to the east} \\ \text{number of steps to the north} \\ \text{number steps up vertical ladder} \end{pmatrix} \] (6-1)

\[ \vec{x} = \begin{pmatrix} 3 \\ 2.4 \\ 1.5 \end{pmatrix} \] determines position \[ \begin{pmatrix} x_{\text{east}} \\ x_{\text{north}} \\ x_{\text{up}} \end{pmatrix} \] (6-2)

The vector above is just one example of a position vector. We could also use coordinate systems that differ from the Cartesian \((x, y, z)\) to represent the location. For example, the location in cylindrical coordinate system could be written as

\[ \vec{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r \cos \theta \\ r \sin \theta \\ z \end{pmatrix} \] (6-3)

as a Cartesian vector in terms of the cylindrical coordinates \((r, \theta, z)\).

The position could also be written as a cylindrical, or polar vector

\[ \vec{x} = \begin{pmatrix} r \\ \theta \\ z \end{pmatrix} = \begin{pmatrix} \sqrt{x^2 + y^2} \\ \tan^{-1} \frac{y}{x} \\ z \end{pmatrix} \] (6-4)
where the last term is the polar vector in terms of the Cartesian coordinates. Similar rules would apply for other coordinate systems like spherical, elliptic, etc.

However, vectors need not represent position at all, for example:

\[
\vec{n} = \left( \begin{array}{c}
\text{number of Hydrogen atoms} \\
\text{number of Helium atoms} \\
\text{number of Lithium atoms} \\
\vdots \\
\text{number of Plutonium atoms} \\
\end{array} \right)
\]  

\text{(6-5)}

\[
\frac{1}{\text{Navag.}} \vec{n} \equiv \left( \begin{array}{c}
\frac{\text{number of H}}{\text{Navag.}} \\
\frac{\text{number of He}}{\text{Navag.}} \\
\frac{\text{number of Li}}{\text{Navag.}} \\
\vdots \\
\frac{\text{number of Pu}}{\text{Navag.}} \\
\end{array} \right) = \left( \begin{array}{c}
\text{moles of H} \\
\text{moles of He} \\
\text{moles of Li} \\
\vdots \\
\text{moles of Pu} \\
\end{array} \right) = \vec{m}
\]  

\text{(6-6)}

\[
\|\vec{x}\| = x_1^2 + x_2^2 + \ldots + x_k^2 = \text{euclidean separation}
\]  

\text{(6-7)}

\[
\|\vec{n}\| = n_H + n_{He} + \ldots + n_{132} = \text{total number of atoms}
\]  

\text{(6-8)}
unit direction vector mole fraction composition
\[ \hat{x} = \frac{x}{\|x\|} \quad \hat{m} = \frac{m}{\|m\|} \]

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**Extra Information and Notes**

*Potentially interesting but currently unnecessary*

If \( \mathbb{R} \) stands for the set of all real numbers (i.e., 0, -1.6, \( \pi/2 \), etc.), then can use a shorthand to specify the position vector, \( \vec{x} \in \mathbb{R}^N \) (e.g., each of the \( N \) entries in the vector of length \( N \) must be a real number—or in the set of real numbers. \( \|\vec{x}\| \in \mathbb{R} \).

For the unit (direction) vector: \( \hat{x} = \{ \vec{x} \in \mathbb{R}^3 \mid \|\vec{x}\| = 1 \} \) (i.e, the unit direction vector is the set of all position vectors such that their length is unity—or, the unit direction vector is the subset of all position vectors that lie on the unit sphere. \( \vec{x} \) and \( \hat{x} \) have the same number of entries, but compared to \( \vec{x} \), the number of independent entries in \( \hat{x} \) is smaller by one.

For the case of the composition vector, it is strange to consider the case of a negative number of atoms, so the mole fraction vector \( \vec{n} \in (\mathbb{R}^+)^{\text{elements}} \) (\( \mathbb{R}^+ \) is the real non-negative numbers) and \( \vec{m} \in (\mathbb{R}^+)^{\text{(elements-1)}} \).

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**Matrices and Matrix Operations**
Consider methane (CH$_4$), propane (C$_3$H$_8$), and butane (C$_4$H$_{10}$).

\[
M_{HC} = \begin{pmatrix}
\text{H-column} & \text{C-column} \\
\text{methane molecule} & \text{methane molecule} \\
\text{number of H} & \text{number of C} \\
\text{number of C} & \text{number of H} \\
\text{propane molecule} & \text{propane molecule} \\
\text{number of H} & \text{number of C} \\
\text{butane molecule} & \text{butane molecule}
\end{pmatrix}
\]

\[
M_{HC} = \begin{pmatrix}
4 & 1 \\
8 & 3 \\
10 & 4
\end{pmatrix} = \begin{pmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22} \\
M_{31} & M_{32}
\end{pmatrix}
\]

\[
N_{HC} = (\text{number of methanes, number of propanes, number of butanes})
\]

\[
= (N_{HC\, m}, N_{HC\, p}, N_{HC\, b})
\]

\[
= (N_{HC\, 1}, N_{HC\, 2}, N_{HC\, 3})
\]
\[ N_{HC}^T M_{HC} \equiv \sum_{i=1}^{3} N_{HC_i} M_{HC_{ij}} = \bar{N} \] (6-17)

The “summation” convention is often used, where a repeated index is summed over all its possible values:
\[ \sum_{i=1}^{p} N_{HC_i} M_{HC_{ij}} \equiv N_{HC_i} M_{HC_{ij}} = N_j \] (6-18)

For example, suppose
\[ N_{HC}^r = (1.2 \times 10^{12} \text{ molecules methane}, 2.3 \times 10^{13} \text{ molecules propane}, 3.4 \times 10^{14} \text{ molecules butane}) \] (6-19)

\[ N_{HC}^r M_{HC} = \]
\[ (1.2 \times 10^{14} \text{ methanes}, 2.3 \times 10^{13} \text{ propanes}, 3.4 \times 10^{12} \text{ butanes}) \]
\[ = (7.0 \times 10^{14} \text{ atoms H, } 2.0 \times 10^{14} \text{ atoms C}) \] (6-20)

\[ N_{HC}^T = \begin{pmatrix} N_{HC_m} \\ N_{HC_p} \\ N_{HC_b} \end{pmatrix} = \begin{pmatrix} N_{HC_m} \\ N_{HC_p} \\ N_{HC_b} \end{pmatrix} \] (6-22)

\[ M_{HC}^T = \begin{pmatrix} \text{methane-column} \\ \text{propane-column} \\ \text{butane-column} \end{pmatrix} \]
\[ \begin{pmatrix} \text{number of H} \\ \text{number of C} \end{pmatrix} \]
\[ \begin{pmatrix} \text{methane molecule} \\ \text{propane molecule} \\ \text{butane molecule} \end{pmatrix} \]
\[ \begin{pmatrix} 4 \text{ atoms H} \\ 8 \text{ atoms H} \\ 10 \text{ atoms H} \end{pmatrix} \]
\[ \begin{pmatrix} \text{methane} \\ \text{propane} \\ \text{butane} \end{pmatrix} \]
\[ \begin{pmatrix} 1 \text{ atoms C} \\ 3 \text{ atoms C} \\ \text{atoms C} \end{pmatrix} \]
\[ \begin{pmatrix} \text{hydrogen row} \\ \text{carbon row} \end{pmatrix} \] (6-21)
\[ M_{HC}^T N_{HC}^T = N^T \begin{pmatrix} 4 & 8 & 10 \\ 1 & 3 & 4 \end{pmatrix} = \begin{pmatrix} \text{number of methanes} \\ \text{number of propanes} \\ \text{number of butanes} \end{pmatrix} = \begin{pmatrix} \text{number of H-atoms} \\ \text{number of C-atoms} \end{pmatrix} \]
Suppose that some process that produces hydrocarbons can be modeled with the pressure $P$ and temperature $T$. Suppose (this is an artificial example) that the number of hydrocarbons produced in one millisecond can be related linearly to the pressure and temperature:

Creating a Matrix

\[
\begin{align*}
\text{number of methanes} &= \alpha P + \beta T \\
\text{number of propanes} &= \gamma P + \delta T \\
\text{number of butanes} &= \epsilon P + \phi T
\end{align*}
\]

or

\[
\mathbf{N}_{HC}^T = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \\ \epsilon & \phi \end{pmatrix} \begin{pmatrix} P \\ T \end{pmatrix}
\]

Then, if we wanted to find an operation that takes us from the processing vector $(P, T)^T$ to the number of hydrogens and carbons:

Matrix multiplication

\[
\mathbf{Q} = \mathbf{M}_{HC}^{-1} \begin{pmatrix} P \\ T \end{pmatrix} = \begin{pmatrix} \text{number of H-atoms} \\ \text{number of C-atoms} \end{pmatrix}
\]

Using matrix multiplication,

\[
\mathbf{Q} = \begin{pmatrix} 4\alpha + 8\gamma + 10\epsilon & 4\beta + 8\delta + 10\phi \\ \alpha + 3\gamma + 4\epsilon & \beta + 3\delta + 4\phi \end{pmatrix}
\]

is a matrix, which when operating on a vector of pressure and temperature, returns a vector of the amount of hydrogen and carbon.
Matrix multiplication is defined by:

\[ AB = \sum_i A_{ki} B_{ij} \]  \hspace{1cm} (6-28)

The indices of the matrix defined by the multiplication \( AB = C \) are \( C_{kj} \).

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**Matrix Inversion** .................................................................

Sometimes what we wish to know, “What vector is it (\( \vec{x} \)), when transformed by some matrix \( (A) \) gives us a particular result (\( \vec{b} = A\vec{x} \))?"

\[
\begin{align*}
A\vec{x} &= \vec{b} \\
A^{-1}A\vec{x} &= A^{-1}\vec{b} \\
\vec{x} &= A^{-1}\vec{b}
\end{align*}
\]  \hspace{1cm} (6-29)

The inverse of a matrix is defined as something that when multiplied with the matrix leaves a product that has no effect on any vector. This special product matrix is called the *identity matrix*. 
Inverting Matrices

Using Inverse[]

\[
Q^{-1} = \frac{1}{\det(Q)} \begin{pmatrix}
-(\beta + 3\delta + 4\phi) & -(2\beta + 4\delta + 5\phi) \\
-(\alpha + 3\gamma + 4\epsilon) & -(2\alpha + 4\gamma + 5\epsilon)
\end{pmatrix}
\]

where

\[
\det(Q) \equiv 4(\alpha\delta - \beta\gamma) - 6(\beta\epsilon - \alpha\phi) + 2(\gamma\phi - \delta\epsilon)
\]

Linear Independence: When solutions exist

\[
\begin{pmatrix}
\mathbf{a}_1 & \mathbf{a}_2
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
= \begin{pmatrix}
b_1 \\
b_2
\end{pmatrix}
\]

(6-32)
Consider liquid water near the freezing point—dipole interactions will tend to make water molecules form clusters such as $\text{H}_2\text{O}$ and $\text{H}_4\text{O}_2$. Then the mapping from molecules to the number of atoms becomes:

$$
\begin{pmatrix}
2 & 4 \\
1 & 2 \\
\end{pmatrix}
\begin{pmatrix}
N_{\text{H}_2\text{O}} \\
N_{\text{H}_4\text{O}_2} \\
\end{pmatrix}
= 
\begin{pmatrix}
N_{\text{H}} \\
N_{\text{O}} \\
\end{pmatrix}
$$

Using RowReduce[]