Sept. 21 2005: Lecture 6:

Linear Algebra I

Reading:
Kreyszig Sections: §6.1 (pp:304–09) , §6.2 (pp:312–18) , §6.3 (pp:321–23) , §6.4 (pp:331–36)

Vectors

Vectors as a list of associated information ....

$$\vec{x} = \begin{pmatrix} \text{number of steps to the east} \\ \text{number of steps to the north} \\ \text{number steps up vertical ladder} \end{pmatrix} \tag{6-1}$$

$$\vec{x} = \begin{pmatrix} 3 \\ 2.4 \\ 1.5 \end{pmatrix} \qquad \text{determines position} \qquad \begin{pmatrix} x_{\text{east}} \\ x_{\text{north}} \\ x_{\text{up}} \end{pmatrix} \tag{6-2}$$

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

$$\vec{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r\cos\theta \\ r\sin\theta \\ z \end{pmatrix} \tag{6-3}$$

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

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

$$\vec{x} = \begin{pmatrix} r \\ \theta \\ z \end{pmatrix} = \begin{pmatrix} \sqrt{x^2 + y^2} \\ \tan^{-1}\frac{y}{x} \\ z \end{pmatrix} \tag{6-4}$$

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:

$$\vec{n} = \begin{pmatrix} \text{number of Hydrogen atoms} \\ \text{number of Helium atoms} \\ \text{number of Lithum atoms} \\ \vdots \\ \text{number of Plutonium atoms} \\ \vdots \end{pmatrix} \tag{6-5}$$

Scalar multiplication ....

$$\frac{1}{\text{N}_{\text{avag.}}}\vec{n} \equiv \begin{pmatrix} \frac{\text{number of H}}{\text{N}_{\text{avag.}}} \\ \frac{\text{number of He}}{\text{N}_{\text{avag.}}} \\ \frac{\text{number of Li}}{\text{N}_{\text{avag.}}} \\ \vdots \\ \frac{\text{number of Pu}}{\text{N}_{\text{avag.}}} \\ \vdots \end{pmatrix} = \begin{pmatrix} \text{moles of H} \\ \text{moles of He} \\ \text{moles of Li} \\ \vdots \\ \text{moles of Pu} \\ \vdots \end{pmatrix} = \vec{m} \tag{6-6}$$

Vector norms ....

$$\|\vec{x}\| \equiv x_1^2 + x_2^2 + \dots x_k^2 = \text{euclidean separation} \tag{6-7}$$

$$\|\vec{n}\| \equiv n_{\text{H}} + n_{\text{He}} + \dots n_{132?} = \text{total number of atoms} \tag{6-8}$$

Unit vectors ....

$$\text{unit direction vector} \qquad \text{mole fraction composition} \tag{6-9}$$

$$\hat{x} = \frac{\vec{x}}{\|\vec{x}\|} \qquad \hat{m} = \frac{\vec{m}}{\|\vec{m}\|} \tag{6-10}$$

Extra Information and Notes

Potentially interesting but currently unnecessary

If $\Re$ 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, $\vec{x} \in \Re^N$ (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. $\|\vec{x}\| \in \Re$.
For the unit (direction) vector: $\hat{x} = \{\vec{x} \in \Re^3 \mid \|\vec{x}\| = 1\}$ (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 $\vec{n} \in (\Re^+)^{elements}$ ($\Re^+$ is the real non-negative numbers) and $\hat{m} \in (\Re^+)^{(elements\text{-}1)}$.

Matrices and Matrix Operations

Consider methane (CH_4), propane (C_3H_8), and butane (C_4H_{10}).

$$\underline{M_{HC}} = \begin{pmatrix} \frac{\text{number of H}}{\text{methane molecule}} & \frac{\text{number of C}}{\text{methane molecule}} \\ \frac{\text{number of H}}{\text{propane molecule}} & \frac{\text{number of C}}{\text{propane molecule}} \\ \frac{\text{number of H}}{\text{butane molecule}} & \frac{\text{number of C}}{\text{butane molecule}} \end{pmatrix} \begin{matrix} \text{methane row} \\ \text{propane row} \\ \text{butane row} \end{matrix} \quad \text{(H-column, C-column)} \tag{6-11}$$

$$\underline{M_{HC}} = \begin{pmatrix} 4 & 1 \\ 8 & 3 \\ 10 & 4 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \\ M_{31} & M_{32} \end{pmatrix} \tag{6-12}$$

Matrices as a linear transformation of a vector . . . .

$$\begin{aligned} \vec{N_{HC}} &= (\text{number of methanes}, \text{number of propanes}, \text{number of butanes}) && \text{(6-13)} \\ &= (N_{HC\,m}, N_{HC\,p}, N_{HC\,b}) && \text{(6-14)} \\ &= (N_{HC\,1}, N_{HC\,2}, N_{HC\,3}) && \text{(6-15)} \\ & && \text{(6-16)} \end{aligned}$$

$$\vec{N_{HC}}\underline{M_{HC}} \equiv \sum_{i=1}^{3} N_{HC\,i} M_{HC\,ij} = \vec{N} \tag{6-17}$$

The "summation" convention is often used, where a repeated index is summed over all its possible values:

$$\sum_{i=1}^{p} N_{HC\,i} M_{HC\,ij} \equiv N_{HC\,i} M_{HC\,ij} = N_j \tag{6-18}$$

For example, suppose

$$\vec{N_{HC}} = (1.2{\times}10^{12} \text{ molecules methane}, 2.3{\times}10^{13} \text{ molecules propane}, 3.4{\times}10^{14} \text{ molecules butane}) \tag{6-19}$$

$$\begin{aligned} &\vec{N_{HC}}\underline{M_{HC}} = \\ &(1.2 \times 10^{14} \text{ methanes}, 2.3 \times 10^{13} \text{ propanes}, 3.4 \times 10^{12} \text{ butanes}) \begin{pmatrix} \frac{\text{4 atoms H}}{\text{methane}} & \frac{\text{1 atoms C}}{\text{methane}} \\ \frac{\text{8 atoms H}}{\text{propane}} & \frac{\text{3 atoms C}}{\text{propane}} \\ \frac{\text{10 atoms H}}{\text{butane}} & \frac{\text{atoms C}}{\text{butane}} \end{pmatrix} \\ =&(7.0 \times 10^{14} \text{ atoms H}, 2.0 \times 10^{14} \text{ atoms C}) \end{aligned} \tag{6-20}$$

Matrix transpose operations . . . .

Above the lists (or vectors) of atoms were stored as rows, often it is convenient to store them as columns. The operation to take a row to a column (and vice-versa) is a "transpose".

$$\underline{M_{HC}}^T = \begin{array}{c} \begin{array}{ccc} \text{methane-column} & \text{propane-column} & \text{butane-column} \end{array} \\ \begin{pmatrix} \frac{\text{number of H}}{\text{methane molecule}} & \frac{\text{number of H}}{\text{propane molecule}} & \frac{\text{number of H}}{\text{butane molecule}} \\ \frac{\text{number of C}}{\text{methane molecule}} & \frac{\text{number of C}}{\text{propane molecule}} & \frac{\text{number of C}}{\text{butane molecule}} \end{pmatrix} \end{array} \begin{array}{c} \text{hydrogen row} \\ \text{carbon row} \end{array} \tag{6-21}$$

$$\vec{N_{HC}}^T = \begin{pmatrix} \text{number of methanes} \\ \text{number of propanes} \\ \text{number of butanes} \end{pmatrix} = \begin{pmatrix} N_{HC\,m} \\ N_{HC\,p} \\ N_{HC\,b} \end{pmatrix} \tag{6-22}$$

$$\underline{M_{HC}}^T \vec{N_{HC}}^T = \vec{N}^T \begin{pmatrix} 4 & 8 & 10 \\ 1 & 3 & 4 \end{pmatrix} \begin{pmatrix} \text{number of methanes} \\ \text{number of propanes} \\ \text{number of butanes} \end{pmatrix} = \begin{pmatrix} \text{number of H-atoms} \\ \text{number of C-atoms} \end{pmatrix} \tag{6-23}$$

Matrix Multiplication ....

MATHEMATICA® Example: Lecture-06

Matrices

Suppose that some process that produces hyrdocarbons 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

$$\begin{aligned}\text{number of methanes} &= \alpha P + \beta T\\ \text{number of propanes} &= \gamma P + \delta T\\ \text{number of butanes} &= \epsilon P + \phi T\end{aligned} \tag{6-24}$$

or

$$\vec{N_{HC}}^T = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \\ \epsilon & \phi \end{pmatrix} \begin{pmatrix} P \\ T \end{pmatrix} \tag{6-25}$$

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

$$\underline{Q} \begin{pmatrix} P \\ T \end{pmatrix} = \underline{M_{HC}}^T \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \\ \epsilon & \phi \end{pmatrix} \begin{pmatrix} P \\ T \end{pmatrix} = \begin{pmatrix} \text{number of H-atoms} \\ \text{number of C-atoms} \end{pmatrix} \tag{6-26}$$

Using matrix multiplication,

$$\underline{Q} = \begin{pmatrix} 4\alpha + 8\gamma + 10\epsilon & 4\beta + 8\delta + 10\phi \\ \alpha + 3\gamma + 4\epsilon & \beta + 3\delta + 4\phi \end{pmatrix} \tag{6-27}$$

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:

$$\underline{AB} = \sum_i A_{ki} B_{ij} \tag{6-28}$$

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

Matrix Inversion

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

$$\begin{aligned} \underline{A}\vec{x} &= \vec{b} \\ \underline{A}^{-1}\underline{A}\vec{x} &= \underline{A}^{-1}\vec{b} \\ \vec{x} &= \underline{A}^{-1}\vec{b} \end{aligned} \tag{6-29}$$

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 *identidy matrix*.

Mathematica® Example: Lecture-04

Inverting Matrices

Using Inverse[]

$$\underline{Q}^{-1} = \frac{1}{\det(\underline{Q})} \begin{pmatrix} -(\beta + 3\delta + 4\phi) & -(2\beta + 4\delta + 5\phi \\ -(\alpha + 3\gamma + 4\epsilon) & -(2\alpha + 4\gamma + 5\epsilon \end{pmatrix} \quad (6\text{-}30)$$

where

$$\det(\underline{Q}) \equiv = 4(\alpha\delta - \beta\gamma) - 6(\beta\epsilon - \alpha\phi) + 2(\gamma\phi - \delta\epsilon) \quad (6\text{-}31)$$

Linear Independence: When solutions exist ....

$$\underline{A}\vec{x} = \vec{b}$$
$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \quad (6\text{-}32)$$

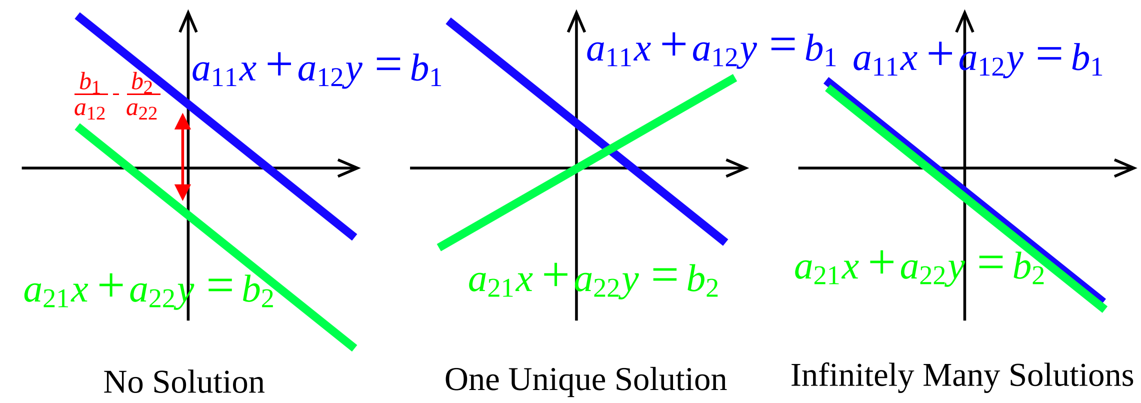

Figure 6-1: Geometric interpretation of solutions in two dimensions

MATHEMATICA® Example: Lecture-06

Eliminating redundant equations or variables

Consider liquid water near the freezing point—dipole interactions will tend to make water molecules form clusters such as H_2O and H_4O_2.
Then the mapping from molecules to the number of atoms becomes:

$$\begin{pmatrix} 2 & 4 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} N_{H_2O} \\ N_{H_4O_2} \end{pmatrix} = \begin{pmatrix} N_H \\ N_O \end{pmatrix} \quad (6\text{-}33)$$

Using RowReduce[]

Linear dependence and the rank of a matrix . . . .