Sept. 17 2012 ____

Lecture 6: Linear Algebra I

Reading:

Kreyszig Sections: 4.0, 7.1, 7.2, 7.3, 7.4, 7.5

Vectors

Vectors as a list of associated information



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 a *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)

i.e., 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

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

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

Scalar multiplication

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

Vector norms

$$\|\vec{x}\| \equiv (x_1^2 + x_2^2 + \dots x_k^2)^{1/2} = \text{euclidean separation (also called l2-norm)}$$
(6-7)
$$\|\vec{n}\| \equiv n_{\text{H}} + n_{\text{He}} + \dots n_{132?} = \text{total number of atoms (related to the Manhatten norm)}$$
(6-8)

Unit vectors

n (6-	mole fraction composition	unit direction vector
(6-1	$\hat{X} = \frac{\vec{N}}{\ \vec{N}\ }$	$\hat{x} = \frac{\vec{x}}{\ \vec{x}\ }$

Matrices and Matrix Operations

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

$$\underline{M}_{HC} = \begin{pmatrix}
\frac{\text{H-column}}{\text{methane molecule}} & \frac{\text{number of C}}{\text{methane molecule}} \\
\frac{\text{number of H}}{\text{propane molecule}} & \frac{\text{number of C}}{\text{propane molecule}} \\
\frac{\text{number of H}}{\text{butane molecule}} & \frac{\text{number of C}}{\text{propane molecule}} \\
\frac{\text{number of H}}{\text{butane molecule}} & \frac{\text{number of C}}{\text{butane molecule}} \\
\frac{M_{HC}}{\text{butane molecule}} = \begin{pmatrix}
4 & 1 \\
8 & 3 \\
10 & 4
\end{pmatrix} = \begin{pmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22} \\
M_{31} & M_{32}
\end{pmatrix}$$
(6-12)

Matrices as a linear transformation of a vector



 $= (N_{HC m}, N_{HC p}, N_{HC b}) \tag{6-14}$

$$= (N_{HC\,1}, N_{HC\,2}, N_{HC\,3}) \tag{6-15}$$

(6-16)

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

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

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

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

Matrix transpose operations

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

$$\underline{M_{HC}}^{T} = \begin{pmatrix} \frac{\text{number of H}}{\text{methane molecule}} & \text{propane-column}\\ \frac{number of H}{\text{methane molecule}} & \frac{number of H}{\text{propane molecule}} & \frac{number of H}{\text{butane molecule}} & \frac{number of H}{\text{butane molecule}} \end{pmatrix} \quad \text{hydrogen row} \quad (6-21)$$

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

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

Matrix Multiplication

The next example supposes that some process produces hydrocarbons and 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:

number of methanes =
$$\alpha P + \beta T$$

number of propanes = $\gamma P + \delta T$ (6-24)
number of butanes = $\epsilon P + \phi T$

or

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

Lecture 06 MATHEMATICA® Example 1

Matrices

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2012.

Here is an example operation that takes us from the processing vector $(P, T)^T$ to the number of hydrogens and carbons.



1: The matrix (Eq. 6-12) is entered as a list of sublists. The sub-lists are the rows of the matrix. The first elements of each row-sublist form the first column; the second elements are the second column and so on.

The Length of a matrix-object gives the number of rows, and the second member of the result of Dimensions gives the number of columns.

All sublists of a matrix must have the same dimensions.

It is good practice to enter a matrix and then display it separately using MatrixForm. Otherwise, there is a risk of defining a symbol as a MatrixForm-object and not as a matrix which was probably the intent.

- 2: The Transpose function exchanges the rows and columns. If Dimensions[Mat] returns {r,c}, then Dimensions[Transpose[Mat]] returns {c,r}.
- 3: Dimensions[PTmatrix] is {3,2}.
- 4: This command will generate an error.

Matrix multiplication in MATHEMATICA® is produced by the "dot" (.) operator—and not the "multiplication" (*) operator. For matrix multiplication, <u>A.B</u>, the number of columns of <u>A</u> must be equal to the number of rows of <u>B</u>.

6: The Transpose "flips" a matrix by producing a new matrix which has the original's ith row as the new matrix's ith column (or, equivalently the jth column as the new jth row). In this example, a 3×2 -matrix (PTmatrix) is being left-multiplied by a a 2×3 -matrix. The resulting matrix would map a vector with values P and T to a vector for the rate of production of C and H.

Matrix multiplication is defined by:

$$\underline{AB} = \sum_{i} A_{ki} B_{ij} \tag{6-26}$$

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

Matrix Inversion

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

$$\underline{A}\vec{x} = \vec{b}$$

$$\underline{A}^{-1}\underline{A}\vec{x} = \underline{A}^{-1}\vec{b}$$

$$\vec{x} = \underline{A}^{-1}\vec{b}$$
(6-27)

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

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2012.

Our last example produced a linear operation that answered the question, "given a particular P and T, at what rate will C and H be produced?"

To answer the converse question, "If I want a particular rate of production for C and H, at what P and T should the process be carried out?"

To invert the question on linear processes, the matrix is inverted.

MPT = Transpose[M _{HC}]. PTmatrix MPTinverse = Factor[Inverse[MPT MPTinverse // MatrixForm	ς; Γ]];	1
$\left(\begin{array}{c} \displaystyle \frac{\beta + 3 \ \bar{\phi} + 4 \ \phi}{2 \ (2 \ \bar{\beta} \ \gamma - 2 \ \alpha \ \bar{\phi} + 3 \ \bar{\phi} + 3 \ \bar{\phi} + \bar{\phi} + 2 \ \alpha \ \bar{\phi} - \gamma \ \phi)} \\ \\ \displaystyle - \frac{\alpha + 3 \ \gamma + 4 \ e}{2 \ (-2 \ \bar{\beta} \ \gamma + 2 \ \alpha \ \bar{\phi} - 3 \ \bar{\beta} \ e - \bar{\delta} \ e + 3 \ \alpha \ \phi + \gamma \ \phi)} \end{array}\right)$	$\frac{2\beta\!+\!4\bar{\sigma}\!+\!5\phi}{2\beta\gamma\!-\!2\alpha\bar{\sigma}\!+\!3\betae\!+\!\bar{\sigma}e\!-\!3\alpha\phi\!-\!\gamma\phi}\\ \frac{2\alpha\!+\!4\gamma\!+\!5e}{-\!2\beta\gamma\!+\!2\alpha\bar{\sigma}\!-\!3\betae\!-\!\bar{\sigma}e\!+\!3\alpha\phi\!+\!\gamma\phi}$)
The denominators are related to the vanishes, then the inverse matrix is no	determinantif the determinated determinated the determinated of	ant
Det[MPT]		2
Checking to see if the the inverse mu identity matrix:	ltiplied by the original matrix is	the
MPT.MPTinverse		3
It is not obvious unless simplified		
Simplify[MPT.MPTinverse] //	MatrixForm	4
$\left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right)$		

- 1: Inverting a matrix by hand is tedious and prone to error, Inverse does this in MATHEMATICA®. In this example, Factor is called on the result of Inverse. Factor is an example of a *threadable function*—it recursively operates on all members of any argument that is a list-object. Thus, each of the entries in the inverted matrix is factored individually.
- 2: The *determinant* of a matrix is fundamentally linked to the existence of its inverse. In this example, it is observed that if the Det of a matrix vanishes, then the entries of its inverse are undetermined.
- **3:** The multiplication of a matrix by its inverse should produce the identity matrix (i.e., a matrix with 1 at each diagonal entry, and zero otherwise). That this multiplication gives the identity matrix is not obvious. Unless, ...
- 4: Simplify is called on each of the entries.

Linear Independence: When solutions exist







Lecture 06 MATHEMATICA® Example 3

Eliminating redundant equations or variables

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2012.

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 .

This example looks at such a case where the columns are not linearly independent.

Same example for water and water complexes: use the matrix w store molecular formulas for each type of molecule in the system	atmat	to
watmat = {{2, 4}, {1, 2}}; watmat // MatrixForm	1	1
The vector molvec is used to store the number of each kind of mo	plecule	
molvec = {h20, h402}	2	
The vector atomvec is used to store the number of each atomic that is present	specie	s
atomvec = {h, o}	3	
atomvec // MatrixForm	4	
The vector eq is now defined and its two elements are equations the number of hydrogen atoms and the number of oxygen atoms:	that gi	ve
eq[1] = (watmat.molvec)[[1]] == atomvec[[1]]	5	2_5
eq[2] = (watmat.molvec)[[2]] == atomvec[[2]]	6	2-0
<pre>Solve[{eq[1], eq[2]}, molvec]</pre>	7	
?Eliminate	8	5-6
Eliminate[eqns, vars] eliminates variables between a set of simultaneous equations. »	ı	
Eliminate[{eq[1], eq[2]}, molvec]	9	7
2 o == h		
MatrixRank[watmat]]10	8-9
NullSpace[watmat] Length[NullSpace[watmat]]	11	
((-2, 1))		10
		U

: The mapping from molecules to the number of atoms becomes:

$$\begin{pmatrix} 2 & 4 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} N_{\mathrm{H}_{2}\mathrm{O}} \\ N_{\mathrm{H}_{4}\mathrm{O}_{2}} \end{pmatrix} = \begin{pmatrix} N_{\mathrm{H}} \\ N_{\mathrm{O}} \end{pmatrix}$$
(6-29)

The matrix watmat encodes the coefficients in these linear equations.

- : The vectors, **atomvec** and **molvec**, represent the numbers of each type of atom and each type of molecule.
- **:** These equations are the same as the rows of $\underline{A}\vec{x}$ being set to the corresponding entry of \vec{b} for $\underline{A}\vec{x} = \vec{b}$. These are the linear equations given above.
- ': This is an attempt (using Solve on the linear equations) to find the number of H_2O - and H_4O_2 -molecules, given the number of Hand O-atoms. Of course, it has to fail.
- **9:** Eliminate produces a logical equality for each redundancy in a set of equations. In this case, the result expresses the fact that $2 \times (\text{second row})$ is the same as the (first row).
- 10: The rank of a matrix, obtained with MatrixRank, gives the number of linearly independent rows.
- 11: The null space of a matrix, \underline{A} , is a linearly independent set of vectors \vec{x} , such that $\underline{A}\vec{x}$ is the zero-vector; this list can be obtained with NullSpace. The result is equivalent to that obtained with Eliminate in item 9. The *nullity* is the number of vectors in a matrix's null space. The rank and the nullity must add up to the number of columns of \underline{A}