Lecture 6: Linear Algebra I

Reading:
Kreyszig Sections: 7.5, 7.6, 7.7, 7.8, 7.9 (pages302–305, 306–307, 308–314, 315–323, 323–329)

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 a *cylindrical coordinate system* could be written as

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

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

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

3.016 Home

Full Screen

Close

Quit

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:

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

Scalar multiplication

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

Vector norms

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

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

3.016 Home

Full Screen

Close

Quit

unit direction vector — mole fraction composition (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 we 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 must be 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 unphysical to have a negative number of atoms, therefore 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}).

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

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

3.016 Home

Full Screen

Close

Quit

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

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

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

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

For example, suppose

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

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

3.016 Home

Full Screen

Close

Quit

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".

$$\underline{M_{HC}}^T = \begin{array}{c} \begin{matrix} \text{methane-column} & \text{propane-column} & \text{butane-column} \end{matrix} \\ \left(\begin{matrix} \frac{\text{number of H}}{\text{methane molecule}} & \frac{\text{number of H}}{\text{propane molecule}} & \frac{\text{number of H}}{\text{butane molecule}} \\ \frac{\text{number of C}}{\text{methane molecule}} & \frac{\text{number of C}}{\text{propane molecule}} & \frac{\text{number of C}}{\text{butane molecule}} \end{matrix} \right) \end{array} \begin{matrix} \text{hydrogen row} \\ \text{carbon row} \end{matrix} \qquad (6\text{-}21)$$

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

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

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:

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

or

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

3.016 Home

Full Screen

Close

Quit

notebook (non-evaluated) pdf (evaluated, color) pdf (evaluated, b&w) html (evaluated)

Matrices

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

M_{HC} is our matrix that maps the three hydrocarbons (methane CH_4, propane C_3H_8, butane C_4H_{10}, to number of hydrogens and carbons

```
MHC = {
    {4, 1},
    {8, 3},
    {10, 4}
  }

MHC // MatrixForm
```
1

```
Transpose[MHC] // MatrixForm
```
2

PTmatrix is our matrix of kinetic data that gives rates of change of a particular atomic species (C or H) as a function of pressure and temperature (see lecture notes corresponding to this Mathematica notebook).

```
PTmatrix = {
     {α, β},
     {γ, δ},
     {ϵ, ϕ}
   };
PTmatrix // MatrixForm
```
3

```
MPT = MHC. PTmatrix
```
4

The matrix multiplication does not work because the sizes are inconsistent.

```
Clear[MPT]
```
5

```
MPT = Transpose[MHC]. PTmatrix;
MPT // MatrixForm
```
6

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, $\underline{A}.\underline{B}$, the number of columns of $\underline{A}$ must be equal to the number of rows of $\underline{B}$.

6: The `Transpose` "flips" a matrix by producing a new matrix which has the original's i^{th} row as the new matrix's i^{th} column (or, equivalently the j^{th} column as the new j^{th} 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.

3.016 Home

Full Screen

Close

Quit

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 ($\vec{b} = \underline{A}\vec{x}$)?"

$$\begin{aligned} \underline{A}\vec{x} &= \vec{b} \\ \underline{A}^{-1}\underline{A}\vec{x} &= \underline{A}^{-1}\vec{b} \\ \vec{x} &= \underline{A}^{-1}\vec{b} \end{aligned} \tag{6-27}$$

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*.

notebook (non-evaluated) pdf (evaluated, color) pdf (evaluated, b&w) html (evaluated)

Inverting Matrices

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
```
1

$$\begin{pmatrix} -\frac{\beta+3\delta+4\phi}{2(2\beta\gamma-2\alpha\delta+3\beta\epsilon+\delta\epsilon-3\alpha\phi-\gamma\phi)} & \frac{2\beta+4\delta+5\phi}{2\beta\gamma-2\alpha\delta+3\beta\epsilon+\delta\epsilon-3\alpha\phi-\gamma\phi} \\ -\frac{\alpha+3\gamma+4\epsilon}{2(-2\beta\gamma+2\alpha\delta-3\beta\epsilon-\delta\epsilon+3\alpha\phi+\gamma\phi)} & \frac{2\alpha+4\gamma+5\epsilon}{-2\beta\gamma+2\alpha\delta-3\beta\epsilon-\delta\epsilon+3\alpha\phi+\gamma\phi} \end{pmatrix}$$

The denominators are related to the determinant---if the determinant vanishes, then the inverse matrix is not defined.

```
Det[MPT]
```
2

Checking to see if the the inverse multiplied by the original matrix is the identity matrix:

```
MPT.MPTinverse
```
3

It is not obvious unless simplified...

```
Simplify[MPT.MPTinverse] // MatrixForm
```
4

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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.

3.016 Home

Full Screen

Close

Quit

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

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{6-28}$$

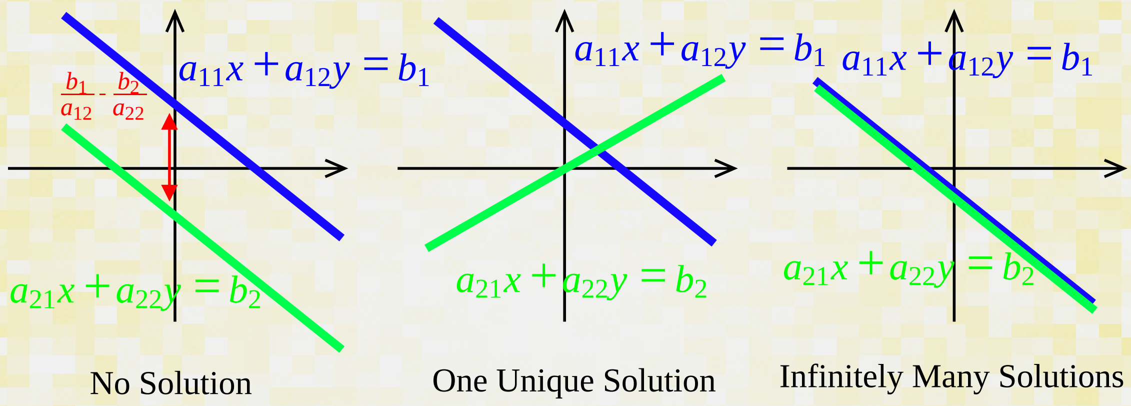

Figure 6-1: Geometric interpretation of solutions in two dimensions

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

Same example for water and water complexes: use the matrix watmat to store molecular formulas for each type of molecule in the system

```
watmat = {{2, 4}, {1, 2}};
watmat // MatrixForm
```
1

The vector molvec is used to store the number of each kind of molecule

```
molvec = {h20, h402}
```
2

The vector atomvec is used to store the number of each atomic species that is present

```
atomvec = {h, o}
```
3

```
atomvec // MatrixForm
```
4

The vector eq is now defined and its two elements are equations that give the number of hydrogen atoms and the number of oxygen atoms:

```
eq[1] = (watmat.molvec)[[1]] == atomvec[[1]]
```
5

```
eq[2] = (watmat.molvec)[[2]] == atomvec[[2]]
```
6

```
Solve[{eq[1], eq[2]}, molvec]
```
7

```
? Eliminate
```
8

Eliminate[*eqns*, *vars*] eliminates variables between a set of simultaneou

```
Eliminate[{eq[1], eq[2]}, molvec]
```
9

```
2 o == h
```

```
MatrixRank[watmat]
```
10

```
NullSpace[watmat]
Length[NullSpace[watmat]]
```
11

```
{{-2, 1}}
```

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

$$\begin{pmatrix} 2 & 4 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} N_{H_2O} \\ N_{H_4O_2} \end{pmatrix} = \begin{pmatrix} N_H \\ N_O \end{pmatrix} \qquad (6\text{-}29)$$

The matrix `watmat` encodes the coefficients in these linear equations.

2–5: The vectors, `atomvec` and `molvec`, represent the numbers of each type of atom and each type of molecule.

5–6: 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.

7: 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 H- and O-atoms. Of course, it has to fail.

8–9: `Eliminate` produces a logical equality for each redundancy in a set of equations. In this case, the result expresses the fact that 2 × (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 $\underline{A}$

3.016 Home

Full Screen

Close

Quit

Index

3.016 Home

Full Screen

Close

Quit

3.016 Home

Full Screen

Close

Quit