Introduction to Matrix Algebra

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Why Learn Matrix Algebra?

- Matrix Algebra is the most popular language of chemometricians.
- Used in chemometrics Texts, Journal Papers and Oral Presentations.
- Need to know Matrix Algebra to stay current with the latest techniques and new ways of applying older techniques.

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Scalar

$$a = 5.4367$$

Just another name for a single number

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Vector

Each member of a Vector is called an Element

$$\mathbf{a} = \underline{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ \bullet \\ \bullet \\ \bullet \\ a_m \end{bmatrix} = \begin{bmatrix} 3.0 \\ -2.1 \\ 9.6 \\ 6.9 \\ 0.4 \\ 8.2 \\ -9.4 \end{bmatrix}$$

Column Vector

up and down

A Vector has Length

Number of Elements or Length = 7

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Transpose to a Row Vector

$$\mathbf{b} = \mathbf{a}^T = [a_1\ a_2\ a_3\ a_4\ a_5\ \bullet\ \bullet\ \bullet\ a_m]$$

$$= [3.0\ \ -2.1\ \ 9.6\ \ 6.9\ \ 0.4\ \ 8.2\ \ -9.4]$$

left and right

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Matrix

$$\mathbf{A} = \underline{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \bullet & \bullet & \bullet & a_{1n} \\ a_{21} & a_{22} & a_{23} & \bullet & \bullet & \bullet & a_{2n} \\ a_{31} & a_{32} & a_{33} & \bullet & \bullet & \bullet & a_{3n} \\ a_{41} & a_{42} & a_{43} & \bullet & \bullet & \bullet & a_{4n} \\ a_{51} & a_{52} & a_{53} & \bullet & \bullet & \bullet & a_{5n} \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ a_{m1} & a_{m2} & a_{m3} & \bullet & \bullet & \bullet & a_{mn} \end{bmatrix}$$

First index is Row Number

Second index is Column Number

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A Matrix is Just a Table of Numbers

	Specific Gravity	App Extr	Alcohol (%w/w)	Real Ext	O.G.	RDF	Calories	pH	Color	IBU	VDK (ppm)
Shea's Irish	1.01016	2.60	3.64	4.29	11.37	63.70	150.10	4.01	19.0	16.1	0.02
Iron Range	1.01041	2.66	3.81	4.42	11.82	64.00	156.30	4.33	11.6	21.1	0.04
Bob's 1st Ale	1.01768	4.50	3.17	5.89	12.04	52.70	162.70	3.93	30.7	21.1	0.11
Manns Original	1.00997	2.55	2.11	3.58	7.77	54.90	102.20	4.05	58.9	18.2	0.05
Killarney's Red	1.01915	4.87	3.83	6.64	14.0	54.30	190.20	4.36	12.3	17.9	0.02
Killian's Irish	1.01071	2.74	3.88	4.48	12.0	64.10	158.80	4.28	53.0	14.2	0.03

6 x 11 Matrix

Rows Columns

Where is a_{37}?

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Transpose a Matrix by Interchanging Rows and Columns

$$\mathbf{B} = \mathbf{A}^T = \begin{bmatrix} 1.2 & 3.5 & -3.1 & 8.6 \\ -0.3 & 8.6 & 0.2 & -4.3 \\ 9.3 & 4.9 & 2.7 & -0.7 \end{bmatrix}^T = \begin{bmatrix} 1.2 & -0.3 & 9.3 \\ 3.5 & 8.6 & 4.9 \\ -3.1 & 0.2 & 2.7 \\ 8.6 & -4.3 & -0.7 \end{bmatrix}$$

3 x 4 Matrix becomes a 4 x 3 Matrix

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The Power of Matrix Algebra is that It Can Perform Operations on a Whole Table of Numbers at Once.

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Matrix Algebra Operations:

Matrix Addition

1.2 + -3.1 = -1.9

$$\mathbf{A} + \mathbf{B} = \begin{bmatrix} 1.2 & 3.5 \\ -0.3 & 8.6 \\ 9.3 & 4.9 \end{bmatrix} + \begin{bmatrix} -3.1 & 8.6 \\ 0.2 & -4.3 \\ 2.7 & -0.7 \end{bmatrix} = \begin{bmatrix} -1.9 & 12.1 \\ -0.1 & 4.3 \\ 12.0 & 4.2 \end{bmatrix}$$

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Matrix Addition is:

- **A** + **B** = **B** + **A** — Commutative
- **A** + (**B** + **C**) = (**A** + **B**) + **C** — Associative

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Scalar Multiplication

2.0 * 1.2 = 2.4

$$k*\mathbf{A} = 2.0 * \begin{bmatrix} 1.2 & 3.5 \\ -0.3 & 8.6 \\ 9.3 & 4.9 \end{bmatrix} = \begin{bmatrix} 2.4 & 7.0 \\ -0.6 & 9.2 \\ 18.6 & 9.8 \end{bmatrix}$$

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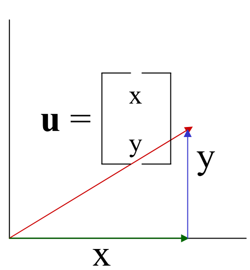
Vector Inner Product (Dot Product)

$$\mathbf{a}^T * \mathbf{b} = [a_1\ a_2\ a_3 \bullet \bullet \bullet\ a_m] * \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_m \end{bmatrix} = \begin{matrix} a_1 b_1 + \\ a_2 b_2 + \\ a_3 b_3 + \\ \vdots \quad + \\ a_m b_m \end{matrix} = \text{Scalar}$$

For an Inner Product to work, **a** and **b** must be the same length.

The Inner Product Can Be Used to Calculate a Vector Length



$$\mathbf{u}^T \mathbf{u} = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = x^2 + y^2$$

According to Pythagorean Theorem

$u^2 = x^2 + y^2$

or the length of **u** is

$u = \|\mathbf{u}\| = (\mathbf{u}^T \mathbf{u})^{1/2}$

Matrix Multiplication

(All Possible Vector Inner Products)

1st Row * 1st Column = 1st Row,1st Column

$$\mathbf{A} * \mathbf{B} = \begin{bmatrix} 1 & 3 & 5 \\ 4 & -2 & 3 \\ 9 & 8 & -3 \end{bmatrix} * \begin{bmatrix} 2 & -3 \\ 8 & 4 \\ -3 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 9 \\ -17 & -20 \\ 11 & 5 \end{bmatrix}$$

3rd Row * 2nd Column = 3rd Row,2nd Column

$$3 \text{ x } 3 * 3 \text{ x } 2 = 3 \text{ x } 2$$

Must be the same

Matrix Multiplication Not Communicative

$$\mathbf{A} * \mathbf{B} \neq \mathbf{B} * \mathbf{A}$$

$$\mathbf{B} * \mathbf{A} = \begin{bmatrix} 2 & -3 \\ 8 & 4 \\ -3 & 0 \end{bmatrix} * \begin{bmatrix} 1 & 3 & 5 \\ 4 & -2 & 3 \\ 9 & 8 & -3 \end{bmatrix} = \begin{bmatrix} ? \end{bmatrix}$$

$$3 \text{ x } 2 * 3 \text{ x } 3$$

Must be the same

Matrix Multiplication is:

- $(\mathbf{A} * \mathbf{B})^T = \mathbf{B}^T * \mathbf{A}^T$
- $(\mathbf{A} + \mathbf{B}) * \mathbf{C} = \mathbf{A} * \mathbf{C} + \mathbf{B} * \mathbf{C}$ $\{\neq \mathbf{C} * \mathbf{A} + \mathbf{C} * \mathbf{B}\}$ Distributive
- $(\mathbf{A} * \mathbf{B}) * \mathbf{C} = A\,(\mathbf{B} * \mathbf{C})$ Associative
- $(\mathbf{A}^T)^T = \mathbf{A}$

Must maintain the order of multiplication!

Another Special Multiplication - Vector Outer Product

(All Possible Scalar Products)

$2 * 4 = 8$

$$\mathbf{a} * \mathbf{b}^T = \begin{bmatrix} 2 \\ 5 \\ 1 \end{bmatrix} \begin{bmatrix} 4 & 3 & 5 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 8 & 6 & 10 & 14 & 18 \\ 20 & 15 & 25 & 35 & 45 \\ 4 & 3 & 5 & 7 & 9 \end{bmatrix}$$

Note: Vector Inner Product resulted in a Scalar

Vector Outer Product resulted in a Matrix

A Special Matrix - Identity Matrix

$$I = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Diagonal Matrix of 1's

Identity Matrix is like the number 1 in Scalar Mathematics

A * I = I * A = A

Both **A** and **I** must be square (m x m) and equal size

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There is No Division in Matrix Algebra

$$\mathbf{A}^{-1} * \mathbf{A} = \mathbf{A} * \mathbf{A}^{-1} = \mathbf{I}$$

Inverse of A

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Not All Matrices Have an Inverse

- They must be square.
- Must not be Collinear.

Collinear - any column (or row) is a linear combination of other columns (or rows).

Other words for Collinear are
Singular and Correlated

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This Matrix is Collinear (Singular)

$$\begin{bmatrix} 2 & 3 & 4 \\ 1 & 0 & 2 \\ 4 & 6 & 8 \end{bmatrix}$$

Simultaneous Equations

$2x + 3y + 4z = 0$

$x + 0 + 2z = 0$

$4x + 6y + 8z = 0$

3rd Row = 1st Row*2

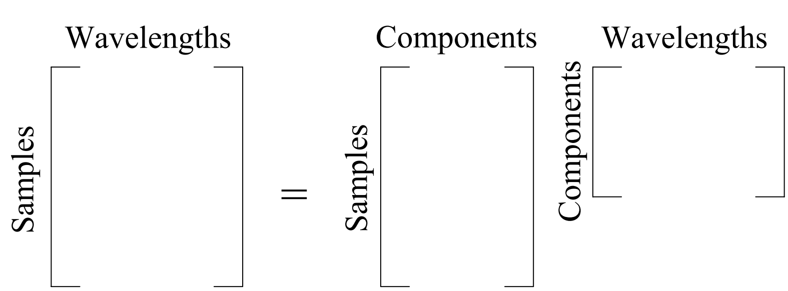
How many unknowns? 3

How many equations? 2

This matrix is not Full Rank   Rank = 2

Beer-Lambert Law

A = **C** **ε**



Solve This Equation for ε

$$A = C\,\varepsilon$$

$$C^{-1} A = C^{-1} C\,\varepsilon$$ But C is usually not square

$$A = C\,\varepsilon$$

$$C^T A = (C^T C)\,\varepsilon$$ $C^T C$ is square

$$\underbrace{(C^T C)^{-1} C^T}_{C^+} A = (C^T C)^{-1} (C^T C)\,\varepsilon = \varepsilon$$

C^+ Moore-Penrose Pseudo Inverse

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Moore-Penrose Pseudo Inverse

- **$(X^T X)^{-1} X^T$** **Use when # rows > # columns**
- **$X^T (X X^T)^{-1}$** **Use when # columns > # rows**
- **X** Must not be Collinear

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The Opposite of Collinear is Orthogonal

Two vectors are Orthogonal (independent) if their inner product $\mathbf{q}_i^T * \mathbf{q}_j = 0$; $i = j$

Other words for Orthogonal are Perpendicular and Independent

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A Matrix is Orthogonal if all the columns are Orthogonal

Special feature of Orthogonal Matrix

$\mathbf{A}^{-1} = \mathbf{A}^T$ if $\mathbf{A}$ is an Orthogonal Matrix

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There are Shades of Grey between Orthogonal and Collinear

2	3	4
1	0	2
4	6	8
5	9	10

2.00	3.00	4.01
1.00	0	2.00
4.01	6.00	7.99
5.02	9.01	10.01

Collinear

With Noise Added
Nearly Collinear

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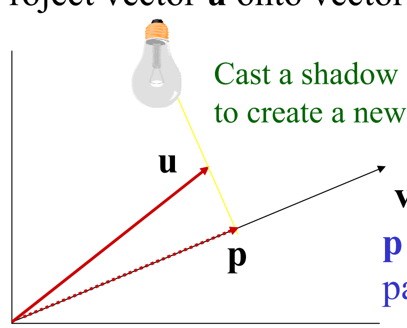
Let's Apply Some of What We Have Learned to Define Projection

Project vector **u** onto vector **v**



Cast a shadow of **u** onto **v** to create a new vector **p**

p is a shortened part of **v**: **p**=b**v**

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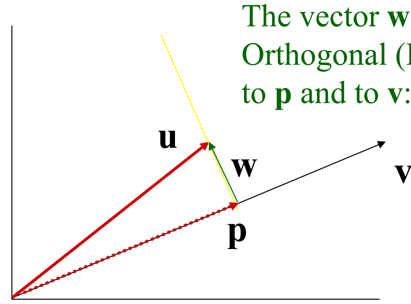
Projection onto a Line



The vector **w** must be Orthogonal (Perpendicular) to **p** and to **v**: $\mathbf{v}^T \mathbf{w} = 0$

w is the vector difference between **u** and **p**: $\mathbf{v}^T (\mathbf{u}-\mathbf{p}) = 0$

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Some Algebra

$\mathbf{v}^T (\mathbf{u}-\mathbf{p}) = 0;$ since $\mathbf{p} = b\mathbf{v}$

$\mathbf{v}^T (\mathbf{u}-b\mathbf{v}) = 0$

solving for **b**

$\mathbf{v}^T \mathbf{u} - \mathbf{v}^T b\mathbf{v} = 0$

$\mathbf{v}^T \mathbf{u} = \mathbf{v}^T b\mathbf{v}$

divide both sides by $\mathbf{v}^T \mathbf{v}$ (Inner Product, a scalar!)

$\mathbf{b} = \mathbf{v}^T \mathbf{u} / \mathbf{v}^T \mathbf{v}$

$\mathbf{p} = (\mathbf{v}^T \mathbf{u} / \mathbf{v}^T \mathbf{v})\mathbf{v}$

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We Shall Teach More Matrix Algebra as We Need It