Linear Algebra for Chemometricians

Outline

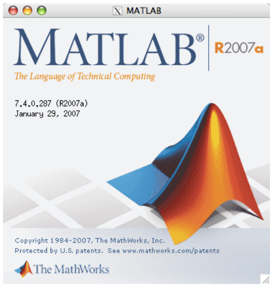
- Definitions
  - scalar, vector, matrix
- Linear Algebra Operations
  - vector and matrix addition
  - vector and matrix multiplication
  - projection
  - Gaussian elimination
  - the concept of rank
  - matrix inverses
  - rank deficiency
- Vector Spaces and Subspaces
- Pseudoinverses
- Singular Value Decomposition

Scalar

- Scalar
- Zero order tensor
- Single number or variable
  - Has a magnitude
  - 1×1
  - Denoted by lower case, $e.g.$ a
  - Temperature, pH, density at single location

Start MATLAB

- We will use MATLAB to demonstrate concepts in linear algebra
- Start MATLAB
- Find Command window (with >> prompt)



Scalars in MATLAB

```
» a = 5;
» a = 5

a =

     5
```


Vector

- Vector
- First order tensor
- Row or column of numbers or variables
  - Has magnitude and direction
  - m × 1 (column) or 1 × n (row)
  - Denoted by bold lower case, *e.g.* **a**
  - Single spectrum, sensor array response

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix}, \quad \mathbf{a}^T = [a_1 \; a_2 \; a_3 \cdots \; a_n]$$

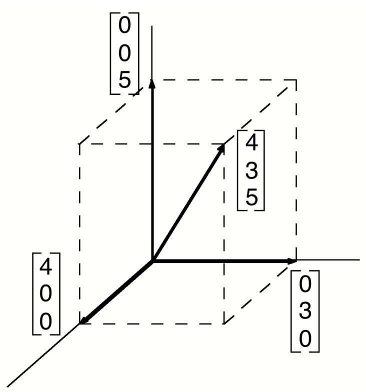
Vectors in MATLAB

```
» b = [4
3
5]

b =

      4
      3
      5
» b = [4; 3; 5];
```


Vector Graphical Representation



Assign vector to another variable

```
» c = b'

c =

   4          3          5
»
```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Matrix

- Matrix
- Second order tensor
- Table or array of numbers or variables
  - m × n, m rows and n columns
  - Denoted by bold upper case, *e.g.* **A**
  - Sprectra of multiple samples, single GC-MS sample

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Matrix (cont.)

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix}$$

$$A = \begin{bmatrix} a & b & c \\ d & e & f \end{bmatrix}$$

$$A^T = \begin{bmatrix} a & d \\ b & e \\ c & f \end{bmatrix}$$

- Matrix and vector transpose
  - Denoted by superscript T or apostrophe ‘
  - Columns of **A** become rows of $\mathbf{A}^T$

Matrices in MATLAB

$$\mathbf{A} = \begin{bmatrix} 2 & 5 & 3 & 6 \\ 7 & 3 & 2 & 1 \\ 5 & 2 & 0 & 3 \end{bmatrix}$$

```
» A = [2 5 3 6; 7 3 2 1; 5 2 0 3];
» A(2,4)

ans =

     1
```

Matrix Transpose

$$\mathbf{A}^T = \begin{bmatrix} 2 & 7 & 5 \\ 5 & 3 & 2 \\ 3 & 2 & 0 \\ 6 & 1 & 3 \end{bmatrix}$$

```
» A'

ans =

     2     7     5
     5     3     2
     3     2     0
     6     1     3
```


Vector and Matrix Addition

- Must be same size
- Addition is element by element

$$\mathbf{a} + \mathbf{b} = \begin{bmatrix} a_1 + b_1 \\ a_2 + b_2 \\ a_3 + b_3 \\ \vdots \\ a_n + b_n \end{bmatrix}$$

Matrix Addition

$$\begin{bmatrix} 1 & 4 & 3 \\ 5 & 4 & 0 \end{bmatrix} + \begin{bmatrix} 2 & 4 & 1 \\ 2 & 6 & 3 \end{bmatrix} = \begin{bmatrix} 3 & 8 & 4 \\ 7 & 10 & 3 \end{bmatrix}$$

```
» x = [1 4 3; 5 4 0]; y = [2 4 1; 2 6 3];
» x + y

ans =

     3     8     4
     7    10     3
```

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Dimensions must be the same!

$$\begin{bmatrix} 1 & 4 & 3 \\ 5 & 4 & 0 \end{bmatrix} + \begin{bmatrix} 2 & 4 \\ 1 & 2 \\ 6 & 3 \end{bmatrix} = ??$$

```
» x = [1 4 3; 5 4 0]; y = [2 4; 1 2; 6 3];
» x + y
??? Error using ==> +
Matrix dimensions must agree.
```

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Vector and Matrix Addition

- Commutative
- Associative

$$\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}$$
$$\mathbf{a} + (\mathbf{b} + \mathbf{c}) = (\mathbf{a} + \mathbf{b}) + \mathbf{c}$$

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Multiplication by a Scalar

- Multiply each element by the scalar
- Similar for matrices and vectors

$$k\mathbf{a}^T = [ka_1\ ka_2\ ka_3 \dots ka_n]$$

- Commutative
- Associative

$$k\mathbf{a} = \mathbf{a}k$$
$$(k+e)\mathbf{a} = k\mathbf{a} + e\mathbf{a}$$

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Scalar Multiplication

$$c = 2, \rightarrow c\mathbf{A} = \begin{bmatrix} 4 & 10 & 6 & 12 \\ 14 & 6 & 4 & 2 \\ 10 & 4 & 0 & 6 \end{bmatrix}$$

```
» c = 2;
» c*A

ans =

     4          10           6          12
    14           6           4           2
    10           4           0           6
```


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Vector Multiplication: Inner Product

- Rectors must have same length
- Result is a scalar

$$\mathbf{a}^T\mathbf{b} = [a_1\ a_2\ a_3 \cdots a_n] \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$

$$\mathbf{a}^T\mathbf{b} = [a_1 b_1 + a_2 b_2 + a_3 b_3 + \ldots + a_n b_n]$$

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Inner Product Example

$$\mathbf{a} = \begin{bmatrix} 2 \\ 5 \\ 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 4 \\ 3 \\ 5 \end{bmatrix}$$

$$\mathbf{a}^T\mathbf{b} = \begin{bmatrix} 2 & 5 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ 3 \\ 5 \end{bmatrix} = \begin{bmatrix} 2*4+5*3+1*5 \end{bmatrix} = 28$$

Also known as "dot product"

Inner Product in MATLAB

```
» a = [2; 5; 1]; b = [4; 3; 5];
» a'*b

ans =

    28
```

Length or "norm" of a Vector

- Square root of the sum of squared elements
- Can be calculated with inner product

$$\|\mathbf{a}\| = \sqrt{\mathbf{a}^T\mathbf{a}}$$

```
» sqrt(a'*a)

ans =

    5.4772

» norm(a)

ans =

    5.4772
```

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Vector Outer Product

- Vectors can have different length
- Result is a matrix

$$\mathbf{ba}^T = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_m \end{bmatrix} [a_1\ a_2\ a_3\ \cdots\ a_n] \qquad \mathbf{ba}^T = \begin{bmatrix} b_1a_1 & b_1a_2 & \cdots & b_1a_n \\ b_2a_1 & b_2a_2 & \cdots & b_2a_n \\ \vdots & \vdots & \ddots & \vdots \\ b_ma_1 & b_ma_2 & \cdots & b_ma_n \end{bmatrix}$$

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Outer Product Example

$$\mathbf{a} = \begin{bmatrix} 2 \\ 5 \\ 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 4 \\ 3 \\ 5 \\ 7 \\ 9 \end{bmatrix}$$

$$\mathbf{ab}^T = \begin{bmatrix} 2 \\ 5 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 4 & 3 & 5 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 2*4 & 2*3 & 2*5 & 2*7 & 2*9 \\ 5*4 & 5*3 & 5*5 & 5*7 & 5*9 \\ 1*4 & 1*3 & 1*5 & 1*7 & 1*9 \end{bmatrix}$$

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

Outer Product in MATLAB

```
» a = [2 5 1]'; b = [4 3 5 7 9]';
» a*b'

ans =

     8     6    10    14    18
    20    15    25    35    45
     4     3     5     7     9
```

Matrix Multiplication

- Size must be compatible
- Order must be maintained

$$\mathbf{A}_{mxn}\mathbf{B}_{nxk} = \mathbf{AB}_{mxk}$$

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}_{3x2} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}_{2x2} = \begin{bmatrix} a_{11}b_{11}+a_{12}b_{21} & a_{11}b_{12}+a_{12}b_{22} \\ a_{21}b_{11}+a_{22}b_{21} & a_{21}b_{12}+a_{22}b_{22} \\ a_{31}b_{11}+a_{32}b_{21} & a_{31}b_{12}+a_{32}b_{22} \end{bmatrix}_{3x2}$$

Matrix Multiplication Example

$$\mathbf{A} = \begin{bmatrix} 2 & 5 & 1 \\ 4 & 5 & 3 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 4 & 3 & 5 & 7 \\ 9 & 5 & 3 & 4 \\ 5 & 3 & 6 & 7 \end{bmatrix}$$

$$\mathbf{AB} = \begin{bmatrix} 2*4+5*9+1*5 & 2*3+5*5+1*3 & 2*5+5*3+1*6 & 2*7+5*4+1*7 \\ 4*4+5*9+3*5 & 4*3+5*5+3*3 & 4*5+5*3+3*6 & 4*7+5*4+3*7 \end{bmatrix}$$

$$\mathbf{AB} = \begin{bmatrix} 58 & 34 & 31 & 41 \\ 76 & 46 & 53 & 69 \end{bmatrix}$$

Multiplication in MATLAB

```
» A = [2 5 1; 4 5 3];
» B = [4 3 5 7; 9 5 3 4; 5 3 6 7];
» A*B

ans =

    58    34    31    41
    76    46    53    69
```


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Matrix Algebra Identities

Matrix multiplication is distributive and associative, but not commutative.

$$(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$$
$$(\mathbf{A}+\mathbf{B})\mathbf{C} = \mathbf{AC} + \mathbf{BC} \neq \mathbf{CA} + \mathbf{CB}$$
$$(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC})$$
$$(\mathbf{A} + \mathbf{B})^T = \mathbf{A}^T + \mathbf{B}^T$$
$$(\mathbf{A}^T)^T = \mathbf{A}$$
$$\mathbf{AI} = \mathbf{IA} = \mathbf{A}$$

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Orthogonal and Orthonormal Vectors

- Vectors orthogonal if inner product is zero
- Orthonormal if orthogonal and unit length, *i.e.* inner product with themselves is 1
- For orthonormal set $\mathbf{v}_i$, with i = 1, 2, … n

$$\mathbf{v}_i^T \mathbf{v}_j = \begin{Bmatrix} 0 \text{ for } i \neq j \\ \hline 1 \text{ for } i = j \end{Bmatrix}$$

- In three dimensions, most common orthonormal basis is $[1\ 0\ 0]^T$, $[0\ 1\ 0]^T$, and $[0\ 0\ 1]^T$

Special Matrices

- Vector is a special matrix (1 row or column)
- Diagonal (non-zero elements on diagonal)
- Identity (square with ones on diagonal)

$$\mathbf{A} = \begin{bmatrix} a_{11} & 0 & 0 & \dots & 0 \\ 0 & a_{22} & 0 & \dots & 0 \\ 0 & 0 & a_{33} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & a_{nn} \end{bmatrix} \qquad \mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Example Special Matrices

$$\mathbf{D} = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 7 & 0 \end{bmatrix} \qquad \mathbf{I}_{4x4} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
» id = eye(3)

id =

     1     0     0
     0     1     0
     0     0     1
```

```
» dm = diag([3 6 9])

dm =

     3     0     0
     0     6     0
     0     0     9
```


Special Matrix Useful Properties

- Any matrix multiplied by identity matrix is unchanged
- Size must be compatible!
- $\mathbf{A}_{mxn}\mathbf{I}_{nxn} = \mathbf{I}_{mxm}\mathbf{A}_{mxn} = \mathbf{A}_{mxn}$
- $(\mathbf{A}^{T})^{-1} = (\mathbf{A}^{-1})^{T}$
- For symmetric matrix **B**, $\mathbf{B} = \mathbf{B}^{T}$
- Symmetric matrices must be square

Solving Systems of Equations

Suppose you have the following system of three equations in three unknowns:

$$\begin{aligned} 2b_1 + b_2 + b_3 &= 1 \\ 4b_1 + b_2 \phantom{{}+b_3} &= -2 \\ -2b_1 + 2b_2 + b_3 &= 7 \end{aligned}$$

This could also be written:

$$\begin{bmatrix} 2 & 1 & 1 \\ 4 & 1 & 0 \\ -2 & 2 & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \\ 7 \end{bmatrix}$$

Or in matrix notation:

$$\mathbf{Xb} = \mathbf{y}$$

Gaussian Elimination

Want to find values of b_1, b_2 and b_3 which make the system hold. Subtract multiples of equations from each other to eliminate variables:

pivot

$$\begin{bmatrix} 2 & 1 & 1 \\ 0 & -1 & -2 \\ 0 & 3 & 2 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -4 \\ 8 \end{bmatrix} \begin{array}{l} \\ \leftarrow \text{Eq 2 - 2*Eq 1} \\ \leftarrow \text{Eq 3 + Eq 1} \end{array}$$

pivot

$$\begin{bmatrix} 2 & 1 & 1 \\ 0 & -1 & -2 \\ 0 & 0 & -4 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -4 \\ -4 \end{bmatrix} \begin{array}{l} \\ \\ \leftarrow \text{Eq 3 + 3*Eq 2} \end{array}$$

From this we see that $b_3 = 1$, and we can use back-substitution to get $b_2 = 2$ and $b_1 = -1$

Gaussian Elimination in MATLAB

```
» X = [2 1 1; 4 1 0; -2 2 1];
» y = [1; -2; 7];
» b = X\y

b =

    -1
     2
     1
```


Inconsistent Systems

Now suppose you have this system:

$$\begin{bmatrix} 1 & 3 & 2 \\ 2 & 6 & 9 \\ 3 & 9 & 8 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -4 \\ -4 \end{bmatrix}$$

Elementary row operations would reduce this to:

pivot

$$\begin{bmatrix} 1 & 3 & 2 \\ 0 & 0 & 5 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -6 \\ -7 \end{bmatrix}$$

This system has no solution as Eq 2 requires that b_3 = -6/5 while Eq 3 requres b_3 = -7/2.

Underdetermined Systems

Suppose instead you started with:

$$\begin{bmatrix} 1 & 3 & 2 \\ 2 & 6 & 9 \\ 3 & 9 & 8 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -8 \\ 1 \end{bmatrix}$$

Elementary row operations would reduce this to:

$$\begin{bmatrix} 1 & 3 & 2 \\ 0 & 0 & 5 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -10 \\ -4 \end{bmatrix}$$

This system has infinitely many solutions, $b_3 = -2$, but $b_1 + 3b_2 = 5$.

Singular Matrices and Rank

Suppose you took an additional step and reduced your matrix to:

$$\begin{bmatrix} 1 & 3 & 2 \\ 2 & 6 & 9 \\ 3 & 9 & 8 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 3 & 2 \\ 0 & 0 & 5 \\ 0 & 0 & 0 \end{bmatrix}$$

This is the *echelon form* of a matrix. It is upper triangular. The number of non-zero rows is the *rank* of the matrix. This can be done on any matrix--it need not be square. It can be shown that:

$$\text{rank}(\mathbf{X}) \leq \min(m,n)$$

A matrix with rank = min(m,n) is said to be of full rank. Otherwise, the matrix is *rank deficient* or *singular*.

Singular Matrices in MATLAB

```
» X = [1 3 2; 2 6 9; 3 9 8];
» y = [1; -8; -1];
» b = X\y

Warning: Matrix is singular to working
  precision.

b =

   -Inf
    Inf
   -2.0000
```


Finding the Rank of a Matrix in MATLAB

- Rank of a matrix is the number of independent rows or columns (same)
- Can think of this as the number of independent variations in the data

```
» rank(X)

ans =

     2
```

Matrix Inverse

- Matrix must be square
- Inverse might not exist!
- If it does exist, matrix is said to be *invertible*
- Matrix must be non-singular *i.e.* full rank
  - no row or column the same as another
  - no row or column a scalar multiple of another
  - no row or column all zeros

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

Orthogonal Matrix

- In the special case of an orthogonal matrix the transpose is the inverse

$$\mathbf{P}^{T}\mathbf{P} = \mathbf{I}$$

$$\mathbf{P}^{-1} = \mathbf{P}^{T}$$

Useful Identities with Inverses

- $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$
- Can be extended to multiple matrices
- $(\mathbf{ABC})^{-1} = \mathbf{C}^{-1}\mathbf{B}^{-1}\mathbf{A}^{-1}$
- Same set of transformations that transform **A** to **I** transform **I** to $\mathbf{A}^{-1}$
- Known as the Gauss-Jordan method

Example of Gauss-Jordan

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 1 \\ 4 & 1 & 0 \\ -2 & 2 & 1 \end{bmatrix}$$

$$\left[\begin{array}{ccc|ccc} 2 & 1 & 1 & 1 & 0 & 0 \\ 4 & 1 & 0 & 0 & 1 & 0 \\ -2 & 2 & 1 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} 2 & 1 & 1 & 1 & 0 & 0 \\ 0 & -1 & -2 & -2 & 1 & 0 \\ 0 & 0 & -4 & -5 & 3 & 1 \end{array}\right]$$

$$\left[\begin{array}{ccc|ccc} 2 & 1 & 0 & \frac{-1}{4} & \frac{3}{4} & \frac{1}{4} \\ 0 & -1 & 0 & \frac{1}{2} & \frac{-1}{2} & \frac{-1}{2} \\ 0 & 0 & -4 & -5 & 3 & 1 \end{array}\right] \qquad \left[\begin{array}{ccc|ccc} 2 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{-1}{4} \\ 0 & -1 & 0 & \frac{1}{2} & \frac{-1}{2} & \frac{-1}{2} \\ 0 & 0 & -4 & -5 & 3 & 1 \end{array}\right]$$

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & \frac{1}{8} & \frac{1}{8} & \frac{-1}{8} \\ 0 & 1 & 0 & \frac{-1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 1 & \frac{5}{4} & \frac{-3}{4} & \frac{-1}{4} \end{array}\right]$$

Gauss-Jordan in MATLAB

```
» format rational
» A = [2 1 1; 4 1 0; -2 2 1];
» B = rref([A eye(3)])

B =

     1         0         0        1/8       1/8      -1/8
     0         1         0       -1/2       1/2       1/2
     0         0         1        5/4      -3/4      -1/4

» A*B(:,4:6)

ans =

     1         0         0
     0         1         0
     0         0         1
```


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Inverse Function in MATLAB

```
» Ainv = inv(A)

Ainv =

    1/8       1/8      -1/8
   -1/2       1/2       1/2
    5/4      -3/4      -1/4

» inv(A') - inv(A)'

ans =

     0            0            0
     0            0            0
     0            0            0
```


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Vector Spaces and Subspaces

- *Vector spaces* denoted $\mathbf{R}^1$, $\mathbf{R}^2$, $\mathbf{R}^3$, … $\mathbf{R}^n$
- Dimension of the space is n
- $\mathbf{R}^3$ is our usual three dimensional space
- $\mathbf{R}^2$ is a planar space
- A *subspace* is a vector space contained within another
- A subspace of a vector space is a subset of the space where:
  - the sum of any two vectors in the subspace is also in the subspace
  - any scalar multiple of a vector in the subspace is also in the subspace.

Linear Independence

- Given a set of vectors $\mathbf{v}_1$, $\mathbf{v}_2$, ... , $\mathbf{v}_k$, if all non-trivial combinations of the vectors are nonzero

  $c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + ... + c_k\mathbf{v}_k \neq 0$ unless $c_1 = c_2 = ... = c_k = 0$

  then the vectors are *linearly independent*. Otherwise, at least one of the vectors is a linear combination of the other vectors and they are *linearly dependent*.

- A set of vectors $\mathbf{w}_1$, $\mathbf{w}_2$, ... , $\mathbf{w}_k$, in $\mathbf{R}^n$ is said to *span the space* if every vector $\mathbf{v}$ in $\mathbf{R}^n$ can be expressed as a linear combination of $\mathbf{w}$'s, *i.e.*

  $\mathbf{v} = c_1\mathbf{w}_1 + c_2\mathbf{w}_2 + ... + c_k\mathbf{w}_k$ for some c_i.

  Note that for the set of $\mathbf{w}$'s to span $\mathbf{R}^n$ then $k \geq n$.

Basis Sets

- A *basis* for a vector space is a set of vectors that are linearly independent and span the space.
  - The number of vectors in the basis must be equal to the dimension of the space.
  - Any vector in the space can be specified as one and only one combination of the basis vectors.
  - Any linearly independent set of vectors can be extended to a basis by adding (linearly independent) vectors so that the set spans the space.
  - Any spanning set of vectors can be reduced to a basis by eliminating linearly dependent vectors.

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Row Spaces and Column Spaces

- For matrix $\mathbf{A}_{mxn}$ of rank r, reduced echelon form $\mathbf{U}$
  - *Row space* is the space spanned by rows of **A**
  - Dimension of the row space, $\mathcal{R}(\mathbf{A}^T)$, equals r
  - Rows of **U** form basis for row space of **A**
  - *Column space* is the space spanned by columns of **A**
  - Dimension of the column space, $\mathcal{R}(\mathbf{A})$, also equals r
  - Columns of **U** (with non-zero pivots) form basis for column space of **A**
- Row rank = column rank!

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Null Spaces

- The *nullspace* of **A**, $\mathcal{N}(\mathbf{A})$, is of dimension n - r. $\mathcal{N}(\mathbf{A})$ is the space of $\mathbf{R}^n$ not spanned by the rows of **A**.
- Likewise, the nullspace of $\mathbf{A}^T$, $\mathcal{N}(\mathbf{A}^T)$, (also known as the left nullspace of **A**) has dimension m - r, and is the space of $\mathbf{R}^m$ not spanned by the columns of **A**.

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Orthogonality of Subspaces

- Vectors, **v**, **w**, orthogonal if inner product zero
- Subspaces V and W are orthogonal if every vector **v** in V is orthogonal to every vector **w** in W
- Thus, for $\mathbf{A}_{mxn}$
  - nullspace $\mathcal{N}(\mathbf{A})$ and the row space $\mathcal{R}(\mathbf{A}^T)$ are orthogonal subspaces of $\mathbf{R}^n$.
  - left nullspace $\mathcal{N}(\mathbf{A}^T)$ and the column space $\mathcal{R}(\mathbf{A})$ are orthogonal subspaces of $\mathbf{R}^m$.
- The *orthogonal complement* of a subspace V of $\mathbf{R}^n$ is the space of all vectors orthogonal to V and is denoted $V^{\perp}$ (pronounced V perp).

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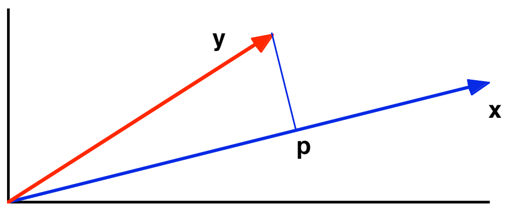
Projections onto Lines

- Projections of points onto lines (also planes and subspaces) very important in chemometrics!
- Projections involve the inner product:

$$\mathbf{p} = \frac{\mathbf{x}^T\mathbf{y}}{\mathbf{x}^T\mathbf{x}} \qquad \text{If } ||\mathbf{x}|| = 1\text{, then } \mathbf{p} = \mathbf{x}^T\mathbf{y}$$



The projection of the vector **y** onto the vector **x**

Derivation of Projection

- Finding **p** is straightforward given that
  - **p** must be a scalar multiple of **x**, *i.e.* **p** = b**x**
  - the line connecting **y** to **p** must be perpendicular to **x**

$$\mathbf{x}^T(\mathbf{y} - b\mathbf{x}) = 0 \rightarrow \mathbf{x}^T\mathbf{y} = b\mathbf{x}^T\mathbf{x} \rightarrow b = \frac{\mathbf{x}^T\mathbf{y}}{\mathbf{x}^T\mathbf{x}}$$

$$\mathbf{p} = b\mathbf{x} = \frac{\mathbf{x}^T\mathbf{y}}{\mathbf{x}^T\mathbf{x}}\mathbf{x}$$

- Also works to project point **y** on subspace **X**, provided that **X** is of rank r = n, i.e. $\mathbf{X}^T\mathbf{X}$ is invertible.

Least Squares

- Consider single variable case with more than 1 equation
  - Want to minimize $E = \|\mathbf{x}b - \mathbf{y}\|$, or the square
  - $E^2 = (\mathbf{x}b - \mathbf{y})^T(\mathbf{x}b - \mathbf{y}) = \mathbf{x}^T\mathbf{x}b^2 - 2\mathbf{x}^T\mathbf{y}b + \mathbf{y}^T\mathbf{y}$
- Take derivative of E^2 wrt b and set to zero

$$\frac{dE^2}{db} = 2\mathbf{x}^T\mathbf{x}b - 2\mathbf{x}^T\mathbf{y} = 0 \rightarrow b = \frac{\mathbf{x}^T\mathbf{y}}{\mathbf{x}^T\mathbf{x}}$$

- Same solution as projection problem!

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Multivariate Least Squares

- Consider $\mathbf{Xb} = \mathbf{y}$ with X_{mxn}, m>n
- Require $\mathbf{Xb} - \mathbf{y}$ be perpendicular to column space of $\mathbf{X}$
- So, each vector in $\mathbf{X}$ must be perpendicular to $\mathbf{Xb} - \mathbf{y}$
- Each vector in column space $\mathbf{X}$ expressible as $\mathbf{Xc}$
- Thus, for all choice of c:
  - $(\mathbf{Xc})^T(\mathbf{Xb} - \mathbf{y}) = 0$, or $\mathbf{c}^T[\mathbf{X}^T\mathbf{Xb} - \mathbf{X}^T\mathbf{y}] = 0$
  - thus, $\mathbf{X}^T\mathbf{Xb} = \mathbf{X}^T\mathbf{y}$ so $\mathbf{b} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
- We often call **b** the regression vector

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Least Squares in MATLAB

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 2 & 1 \\ 2 & 2 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 6 \\ 6 \\ 7 \\ 11 \end{bmatrix}$$

```
» X = [1 1; 1 2; 2 1; 2 2];
» y = [6 6 7 11]';
» b = inv(X'*X)*X'*y

b =

    3.0000
    2.0000
```

```
» b = X\y

b =

    3.0000
    2.0000
```


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Projection of y onto X, orthogonality of residuals

```
» p = X*b

p =

     5
     7
     8
    10

» d = y-p

d =

     1
    -1
    -1
     1
```

```
» X'*d

ans =

   1.0e-14 *

   -0.9770
   -0.9770
```


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Least Squares Summary

- When $m>n$ the system of equations $\mathbf{Xb} = \mathbf{y}$ is overdetermined and the method of least squares can be used to determine $\mathbf{b}$

$$\mathbf{b} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- $\mathbf{X}^T\mathbf{X}$ is square (nxn) but the inverse won't exist if it's not full rank (*i.e.* if rank($\mathbf{X}$) < n)
- What if it's nearly rank deficient?...

Ill-conditioned Matrices

- Suppose that there are two systems of equations with $\mathbf{X}$ nearly rank deficient and differ by only a small amount (as might be expected from data with noise)

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \\ 4 & 8.0001 \end{bmatrix} \quad y_1 = \begin{bmatrix} 2 \\ 4 \\ 6.0001 \\ 8 \end{bmatrix} \quad > \quad b_1 = \begin{bmatrix} 3.71 \\ -0.86 \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \\ 4 & 8.0001 \end{bmatrix} \quad y_2 = \begin{bmatrix} 2 \\ 4 \\ 5.9999 \\ 8 \end{bmatrix} \quad > \quad b_2 = \begin{bmatrix} 0.29 \\ 0.86 \end{bmatrix}$$

- Small changes in $\mathbf{y}$ (and/or $\mathbf{X}$) can have a significant impact on the regression results for nearly rank deficient systems

MATLAB on Similar Example

```
» X = [1 2; 2 4; 3 6; 4 8.0001]; y = [2 4 6 8]';
» b = X\y

b =

     2
     0

» X = [1 2; 2 4; 3 6; 4 8.0001]; y = [2 4 6.0001 8]'; b = X\y

b =

    3.7143
   -0.8571

» X = [1 2; 2 4; 3 6; 4 8.0001]; y = [2 4 5.9999 8]'; b = X\y

b =

    0.2857
    0.8571
```


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Projection Matrices

- For problem $\mathbf{Xb} = \mathbf{y}$, projection of $\mathbf{y}$ onto columns of $\mathbf{X}$, $\mathbf{p}$ was:

$$\mathbf{p} = \mathbf{X}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y},\ \mathbf{p} = \mathbf{P}\mathbf{y}$$

- $\mathbf{P}$ is a *projection matrix*, and is
  - *Idempotent*, *i.e.* $\mathbf{PP} = \mathbf{P}^2 = \mathbf{P}$
  - *Symmetric*, *i.e.* $\mathbf{P}^{\mathrm{T}} = \mathbf{P}$

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Orthogonal and Orthonormal Bases

- Orthonormal basis, $\mathbf{v}_1, \mathbf{v}_2 \ldots \mathbf{v}_k$ has property

$$\mathbf{v}_i^T \mathbf{v}_j = \begin{Bmatrix} 0 \text{ for } i \neq j \\ \hline 1 \text{ for } i = j \end{Bmatrix}$$

- Project $\mathbf{y}$ onto $\mathbf{X}$ with orthonormal columns, so $\mathbf{X}^T\mathbf{X} = \mathbf{I}$

$$\mathbf{P} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T = \mathbf{X}\mathbf{X}^T$$

- Square matrix with orthonormal columns is called an *orthogonal matrix*

Orthogonal Matrix Properties

- For an orthogonal matrix $\mathbf{Q}$ (orthonormal columns)

$$\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$$
$$\mathbf{Q}\mathbf{Q}^T = \mathbf{I}$$
$$\mathbf{Q}^T = \mathbf{Q}^{-1}$$

- Q will also have orthonormal rows!

Pseudoinverses

- How to sove $\mathbf{Xb} = \mathbf{y}$ if $\mathbf{X}^T\mathbf{X}$ singular?
- Introduce pseudoinverse, $\mathbf{X}^+$
- Many solutions, which to choose?
- One that minimizes length of **b**, $||\mathbf{b}||$
- Require that **b** lie in the row space of **X**
  - **Xb** equals projection of **y** into the column space of **X**
  - b lies in the row space of **X**.
- Must find a way to calculate $\mathbf{X}^+$

Singular Value Decomposition

- Any *m* by *n* matrix **X** can be factored into

$$\mathbf{X} = \mathbf{USV}^T$$

U orthogonal and *m* by *m*

V orthogonal and *n* by *n*

S diagonal and *m* by *n*

- Non-zero elements of **S** are singular values and decrease from upper left to lower right

Example SVD

```
» X = [1 2 3; 2 3 5; 3 5 8; 4 8 12];
» [U,S,V] = svd(X)

U =

    0.1935    0.1403   -0.9670    0.0885
    0.3184   -0.6426    0.0341    0.6961
    0.5119   -0.5022   -0.0341   -0.6961
    0.7740    0.5614    0.2503    0.1519

S =

   19.3318         0         0
         0    0.5301         0
         0         0    0.0000
         0         0         0


V =

    0.2825   -0.7661    0.5774
    0.5221    0.6277    0.5774
    0.8047   -0.1383   -0.5774
```

$$X = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 5 \\ 3 & 5 & 8 \\ 4 & 8 & 12 \end{bmatrix}$$

Verify SVD

```
» U*S*V'

ans =

    1.0000    2.0000    3.0000
    2.0000    3.0000    5.0000
    3.0000    5.0000    8.0000
    4.0000    8.0000   12.0000
```

- Note that last singular value appears to be zero!

Formation of the Pseudoinverse

- Recall inverse of a product is product of inverses in reverse order, thus

$$\mathbf{X}^{+} = \mathbf{V}\mathbf{S}^{+}\mathbf{U}^{T}$$

- Remember, **U** and **V** are orthogonal!
- How to form $\mathbf{S}^{+}$?
- Set singular values close to zero to zero in the inverse or truncate the matrices r = rank(**X**) columns

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Reconstruction with two Factors

```
» U(:,1:2)*S(1:2,1:2)*V(:,1:2)'

ans =

    1.0000    2.0000    3.0000
    2.0000    3.0000    5.0000
    3.0000    5.0000    8.0000
    4.0000    8.0000   12.0000
```


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Pseudoinverse Calculation

```
» Xinv = V(:,1:2)*inv(S(1:2,1:2))*U(:,1:2)'

Xinv =

   -0.2000    0.9333    0.7333   -0.8000
    0.1714   -0.7524   -0.5810    0.6857
   -0.0286    0.1810    0.1524   -0.1143
» pinv(X)

ans =

   -0.2000    0.9333    0.7333   -0.8000
    0.1714   -0.7524   -0.5810    0.6857
   -0.0286    0.1810    0.1524   -0.1143
```


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Return to our Ill-Conditioned Problem

$$\mathbf{X} = \begin{bmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \\ 4 & 8.0001 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 2 \\ 4 \\ 6 \\ 8 \end{bmatrix}$$

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Solution

```
» X = [1 2; 2 4; 3 6; 4 8.0001]; y = [2 4 6 8]';
» [U,S,V] = svd(X);
» Xinv = V(:,1)*inv(S(1,1))*U(:,1)'

Xinv =

    0.0067    0.0133    0.0200    0.0267
    0.0133    0.0267    0.0400    0.0533

» b = Xinv*y

b =

    0.4000
    0.8000
```


Solution no Longer Sensitive to Minor Changes

```
» y = [2 4 5.9999 8]';
» b = Xinv*y

b =

    0.4000
    0.8000

» y = [2 4 6.0001 8]';
» b = Xinv*y

b =

    0.4000
    0.8000
```

Inverse stabilized!

Higher Order Tensors

- Arrays can be extended beyond conventional tables, e.g. to 3-D arrays
- Third, fourth, fifth… order tensors
- Usually denoted by bold upper case with underline, *e.g.* $\underline{\mathbf{A}}$
- Collection of samples from GC-MS, batch runs

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Algebra of Higher Order Tensors

- Not as well defined as conventional linear algebra
- Addition and scalar multiplication as expected
- Multiplication of tensors definitions not universally accepted

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Summary

- Basic vector and matrix operations
  - addition and subtraction
  - multiplication
  - vector inner and outer products
- Matrix rank
  - number of independent rows or columns (same)
  - rank ≤ min{m,n} (number of rows and columns)
  - found by reducing to echelon form
- Matrix inverses
  - exist only for square matrices
  - do not exist for rank deficient matrices
- Least squares
  - used to solve inconsistent systems
  - solution unstable in nearly collinear systems
- Singular Value Decomposition and Pseudoinverses

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