Linear Algebra for Chemometricians

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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

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Scalar

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

- Scalar in MATLAB

```
» a = 5;
» a = 5
a =
     5
```


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Vector

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

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix} \qquad \mathbf{a}^T = [a_1\ a_2\ \dots\ a_n]$$

- Vectors in MATLAB

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

» b = [4; 3; 5];
```


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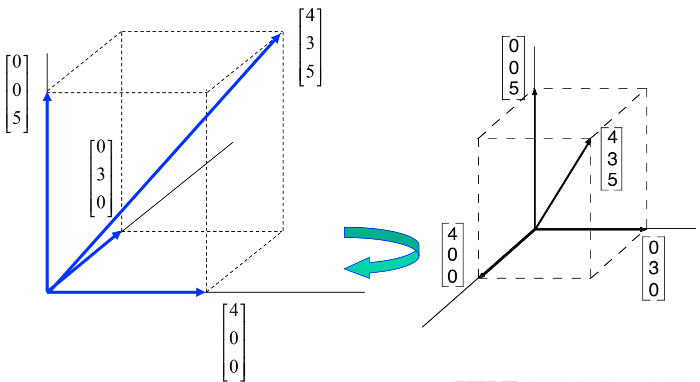
Vector Graphical Representation



Assign vector to another variable

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


Matrix

- Matrix
- Second order tensor
- Table or array of numbers or variables
  - Size m x n, m rows and n columns
  - Denoted by bold upper case, *e.g.* **A**
  - Spectra of multiple samples, multiple process measurements from a batch or continuous process, a single GC-MS sample

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 $\mathbf{A}^T$

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

Where is a_{37}?

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Matrices in MATLAB

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

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

```
» A'
ans =
     2     7     5
     5     3     2
     3     2     0
     6     1     3
```


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Special Matrices

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

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

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Example - Special Matrices

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

```
» id = eye(4)
id =
     1     0     0     0
     0     1     0     0
     0     0     1     0
     0     0     0     1
```

```
» dm = diag([3 6 9])
dm =
     3     0     0
     0     6     0
     0     0     9
```


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Another Word – Diagonal Matrices

```
0     2     0     0     0     0
0     0     4     0     0     0
0     0     0     6     0     0
0     0     0     0     8     0
0     0     0     0     0    10
0     0     0     0     0     0
```

This is a diagonal matrix

And so is this

```
0     0     0     0     0     0
0     0     0     0     0     0
0     0     0     0     0     0
1     0     0     0     0     0
0     3     0     0     0     0
0     0     5     0     0     0
```

First matrix: `dm = diag([2 4 6 8 10],1)`

Second matrix: `dm = diag([1 3 5],-3)`

k^{th} diagonal

Vector and Matrix Addition

- Must be same size
- Addition is element by element

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

- Commutative
- Associative

$$\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}$$

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

Matrix Addition

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

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

dimensions must be the same!

```
» x = [1 4 3; 5 4 0];
» y = [2 4 1; 2 6 3];
» x + y
ans =
       3           8           4
       7          10           3
```

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


Multiplication by a Scalar

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

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

- Commutative
- Associative

$$k\mathbf{a} = \mathbf{a}k$$

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

Scalar Multiplication

$$\mathbf{A} = \begin{bmatrix} 2 & 5 & 3 & 6 \\ 7 & 3 & 2 & 1 \\ 5 & 2 & 0 & 3 \end{bmatrix} \qquad c = 2, \rightarrow c\mathbf{A} = \begin{bmatrix} 4 & 10 & 6 & 12 \\ 14 & 6 & 4 & 2 \\ 10 & 4 & 0 & 6 \end{bmatrix}$$

```
» 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

- Vectors must have same number of elements
- Result is a scalar
- Dot Product

$$\mathbf{a}^T\mathbf{b} = \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ . \\ . \\ . \\ b_n \end{bmatrix}$$

$$\mathbf{a}^T\mathbf{b} = \begin{bmatrix} a_1 b_1 & a_2 b_2 & \dots & a_n b_n \end{bmatrix}$$

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Inner Product Example

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

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

$$= \begin{bmatrix} 2 \cdot 4 + 5 \cdot 3 + 1 \cdot 5 \end{bmatrix} = 28$$

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

ans =
     28
```


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Length or "norm" of a Vector

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

$$\|\mathbf{a}\| = \left(\mathbf{a}^T\mathbf{a}\right)^{1/2} = \left[a_1 a_1 + a_2 a_2 + \dots + a_n a_n\right]^{1/2}$$

```
» 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

$$\mathbf{a}_{mx1}\mathbf{b}^T_{1xn} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} \begin{bmatrix} b_1 & b_2 & \dots & b_n \end{bmatrix} \quad \mathbf{ab}^T = \begin{bmatrix} a_1b_1 & a_1b_2 & \dots & a_1b_n \\ a_2b_1 & a_2b_2 & \dots & a_2b_n \\ \dots & \dots & \ddots & \dots \\ a_mb_1 & a_mb_2 & \dots & a_mb_n \end{bmatrix}$$

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 (inner dimensions must be same)
- Order must be maintained

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

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

Interpretation

- There are a number of ways to interpret/envision matrix multiplication
  - Each element in the resultant matrix is the resultant of the vector/dot product of row and column vectors
    - AB_{ij} = (row i of A) • (column j of B)
  - Each row in AB is a linear combination of the rows in B
  - Each column in AB is a linear combination of the columns in A

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Matrix Multiplication Example

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

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

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Matrix Multiplication Example

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

row 2 column 2

$$\begin{bmatrix} 4 & 5 & 3 \end{bmatrix} \begin{bmatrix} 3 \\ 5 \\ 3 \end{bmatrix} = 46$$

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

element 2,2

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Matrix Multiplication Example

$$A = \begin{bmatrix} 2 & 5 & 1 \\ \boxed{4 \quad 5 \quad 3} \end{bmatrix} \text{ row 2} \quad B = \begin{bmatrix} 4 & 3 & 5 & 7 \\ 9 & 5 & 3 & 4 \\ 5 & 3 & 6 & 7 \end{bmatrix}$$

$$4 * \begin{bmatrix} 4 & 3 & 5 & 7 \end{bmatrix} + $$
$$5 * \begin{bmatrix} 9 & 5 & 3 & 4 \end{bmatrix} + \quad \begin{bmatrix} 76 & 46 & 53 & 69 \end{bmatrix}$$
$$3 * \begin{bmatrix} 5 & 3 & 6 & 7 \end{bmatrix} = $$

$$AB = \begin{bmatrix} 58 & 34 & 31 & 41 \\ \boxed{76 \quad 46 \quad 53 \quad 69} \end{bmatrix} \text{ row 2}$$

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Matrix Multiplication Example

column 3

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

$$5 * \begin{bmatrix} 2 \\ 4 \end{bmatrix} + 3 * \begin{bmatrix} 5 \\ 5 \end{bmatrix} + 6 * \begin{bmatrix} 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 31 \\ 53 \end{bmatrix}$$

column 3

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

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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

$(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$

$(\mathbf{A}+\mathbf{B})\mathbf{C} = \mathbf{AC}+\mathbf{BC} \neq \mathbf{CA}+\mathbf{CB}$

$(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC})$

$(\mathbf{A}+\mathbf{B})^T = \mathbf{A}^T+\mathbf{B}^T$

$(\mathbf{A}^T)^T = \mathbf{A}$

$\mathbf{B} = \mathbf{B}^T$ if **B** symmetric and square

$\mathbf{I}_{MxM}\mathbf{A}_{MxN} = \mathbf{A}_{MxN}\mathbf{I}_{NxN} = \mathbf{A}_{MxN}$ Multiplication by the identity leaves a matrix unchanged

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Solving Systems of Equations

consider the following system of three equations with three unknowns:

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

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

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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:

$$\begin{bmatrix} 2 & 1 & 1 \\ 0 & -1 & -2 \\ 0 & 3 & 2 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -4 \\ 8 \end{bmatrix} \quad \begin{matrix} \\ \text{Eq 2 – 2*Eq 1} \\ \text{Eq 3 + Eq 1} \end{matrix}$$

pivot

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

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

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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
```


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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:

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

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

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Underdetermined Systems

Suppose instead that 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: $b_3 = -2$, and $b_1 + 3b_2 = 5$.

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Singular Matrices and Rank

With an additional step the matrix reduces 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 the matrix. It is upper triangular and the number of non-zero rows is the *rank* of the matrix. Row reduction can be performed on any matrix – it need not be square.

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

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

```
» X = [1 3 2; 2 6 9; 3 9 8];
» rank(X)
ans =
     2
```


Matrix Inverse

- Matrix must be square
- 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 (columns are orthogonal and of unit length) the transpose is the inverse

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

Matrix Inverse Identities

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$$

$$(\mathbf{ABC})^{-1} = \mathbf{C}^{-1}\mathbf{B}^{-1}\mathbf{A}^{-1}$$

- Extensible to multiple matrices

$$[\mathbf{A} \,|\, \mathbf{I}] \rightarrow [\mathbf{I} \,|\, \mathbf{A}^{-1}]$$

- Same set of transformations that transform **A** to **I** transform **I** to $\mathbf{A}^{-1}$
  - Known as the Gauss-Jordan method

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

Example of Gauss-Jordan

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

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

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

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

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

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

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
```


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
```

Vector Spaces and Subspaces

- *Vector spaces* denoted $\mathbf{R}^1, \mathbf{R}^2, \mathbf{R}^3, \ldots \mathbf{R}^n$
- Dimension of the space is n
- $\mathbf{R}^3$ is the familiar 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 subspace contains the zero vector
  - 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.

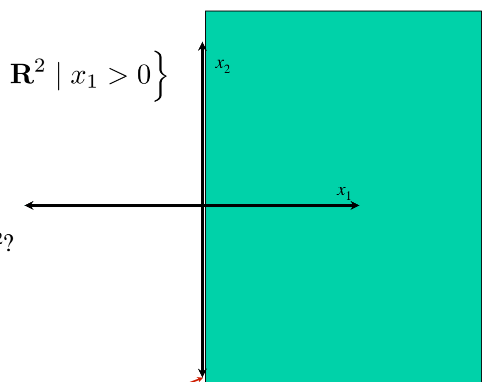
Example: R^3

- The list of all possible subspaces of $\mathbf{R}^3$
  - Any line through [0 0 0]
  - Any plane through [0 0 0]
  - The single vector [0 0 0]
  - The whole space: $\mathbf{R}^3$

Example: R^2

$$S = \left\{ \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbf{R}^2 \mid x_1 > 0 \right\}$$

Is S a subspace of $\mathbf{R}^2$?

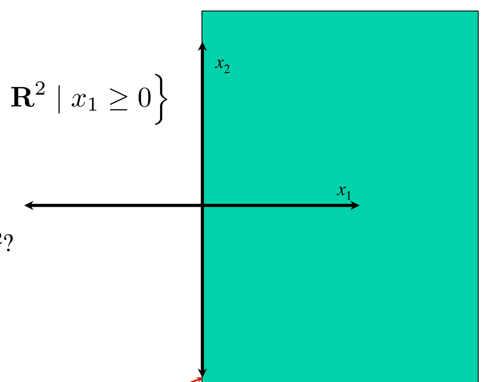


does not include x_2 axis

Example: R^2

$$S = \left\{ \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbf{R}^2 \mid x_1 \geq 0 \right\}$$

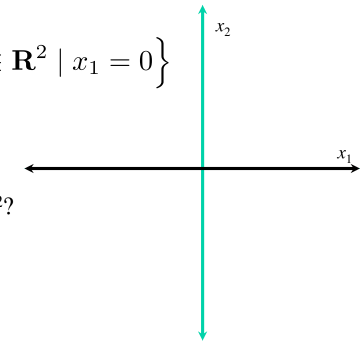
Is S a subspace of $\mathbf{R}^2$?



includes x_2 axis

Example: R^2

$$S = \left\{ \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbf{R}^2 \mid x_1 = 0 \right\}$$



Is S a subspace of $\mathbf{R}^2$?

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Linear Independence

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

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

  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 $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_k$, 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.*

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

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

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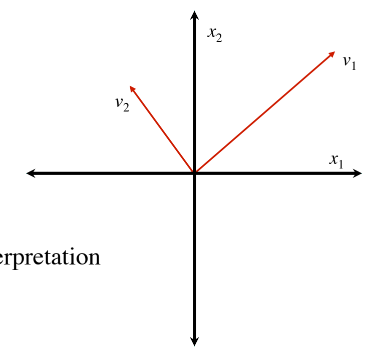
Linear Independence



Geometric interpretation

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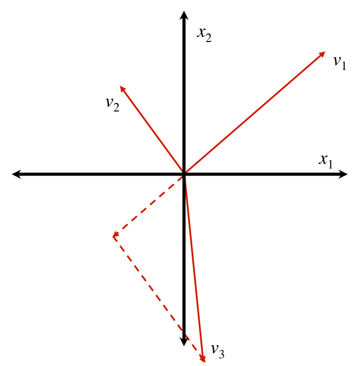
Linear Independence



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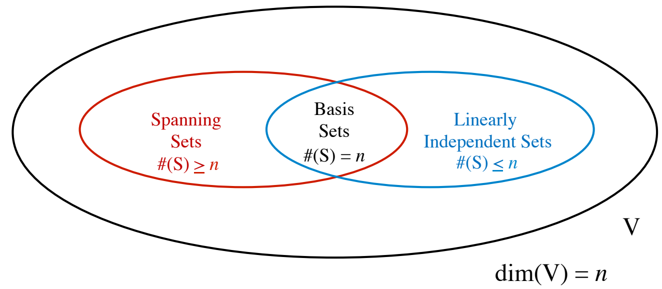
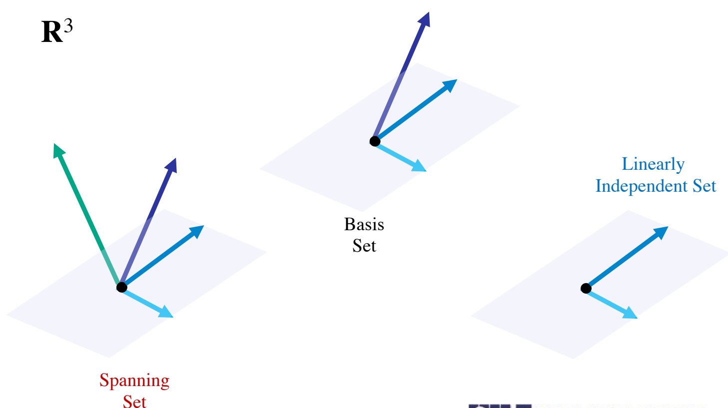
Basis Sets

- 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.

Basis, Spanning, and Linearly Independent Sets



Example



Orthogonal and Orthonormal Bases

- Orthonormal basis, $\mathbf{v}_1, \mathbf{v}_2 \ldots \mathbf{v}_k$ has property
  - Vectors are orthogonal if their inner product is 0
  - Orthonormal if they are both orthogonal and unit length, *i.e.* inner product with themselves is 1

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

- 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)

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

- $\mathbf{Q}$ will also have orthonormal rows!

Row Spaces and Column Spaces

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

Null Spaces

- The *nullspace* of $\mathbf{A}$, $\mathcal{N}(\mathbf{A})$, is of dimension $n - r$. $\mathcal{N}(\mathbf{A})$ is the space of $\mathbf{R}^n$ not spanned by the rows of $\mathbf{A}$.
- Likewise, the nullspace of $\mathbf{A}^{\mathrm{T}}$, $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$, (also known as the left nullspace of $\mathbf{A}$) has dimension $m - r$, and is the space of $\mathbf{R}^m$ not spanned by the columns of $\mathbf{A}$.
- The nullspace of A consists of all solutions to $\mathbf{Ax} = \mathbf{0}$

Orthogonality of Subspaces

- Vectors, $\mathbf{v}$, $\mathbf{w}$, orthogonal if inner product zero
- Subspaces V and W are orthogonal if every vector $\mathbf{v}$ in V is orthogonal to every vector $\mathbf{w}$ in W
- Thus, for $\mathbf{A}_{m\times n}$
  - "right" nullspace $\mathcal{N}(\mathbf{A})$ and the row space $\mathcal{R}(\mathbf{A}^{\mathrm{T}})$ are orthogonal subspaces of $\mathbf{R}^n$.
  - left nullspace $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ 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).

Important Point

- If $\mathbf{V}$ is a subspace of $\mathbf{R}^n$, then $\mathbf{V}^\perp$ is also a subspace of $\mathbf{R}^n$
- Given $\vec{x} \in \mathcal{R}^n$

$$\vec{x} = \vec{v} + \vec{w} \text{ where } \vec{v} \in \mathbf{V} \ \& \ \vec{w} \in \mathbf{V}^\perp$$

$$\operatorname*{Proj}_{\mathbf{V}}(\vec{x}) = \vec{v} \qquad \operatorname*{Proj}_{\mathbf{V}^\perp}(\vec{x}) = \vec{w}$$

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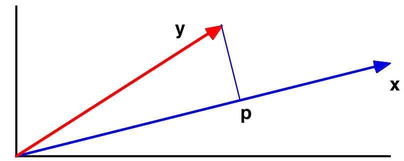
Projections onto Lines

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

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

if $||\mathbf{x}|| = 1$ then $b = \mathbf{x}^\mathrm{T}\mathbf{y}$ and $\mathbf{p} = b\mathbf{x}$



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

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Derivation of Projection

- Finding **p** is straightforward given that
  - **p** must be a scalar multiple of **x**, *i.e.* $\mathbf{p} = b\mathbf{x}$
  - 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. $\mathbf{X}^\mathrm{T}\mathbf{X}$ is invertible.

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Least Squares

- Consider single variable case with more than 1 equation
  - Want to minimize $\mathbf{e}^\mathrm{T}\mathbf{e} = ||\mathbf{x}b - \mathbf{y}||^2$
  - $e^2 = \mathbf{e}^\mathrm{T}\mathbf{e} = (\mathbf{x}b - \mathbf{y})^\mathrm{T}(\mathbf{x}b - \mathbf{y}) = \mathbf{x}^\mathrm{T}\mathbf{x}b^2 - 2\mathbf{x}^\mathrm{T}\mathbf{y}b + \mathbf{y}^\mathrm{T}\mathbf{y}$
- 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 **Xb** = **y** with $X_{m\times n}$, *m>n*
- Require **Xb** - **y** be perpendicular to column space of **X**
- So, each vector in **X** must be perpendicular to **Xb** - **y**
- Each vector in column space **X** expressible as **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 $\mathbf{b} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
- **b** is often called the regression vector

Projection Matrices

- For problem **Xb** = **y**, projection of **y** onto columns of **X**, **p** was:

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

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

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
```


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
```

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 **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(**X**) < n)
- What if it's nearly rank deficient?...

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Ill-conditioned Matrices

- Consider two systems of equations with **X** nearly rank deficient and differing 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 **y** (and/or **X**) can have a significant impact on regression results for nearly rank deficient systems
- A problem for some regression approaches and an opportunity for others!

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MATLAB - 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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Pseudoinverses

- How to solve $\mathbf{Xb} = \mathbf{y}$ if $\mathbf{X}^T\mathbf{X}$ singular?
- Introduce pseudoinverse, $\mathbf{X}^+$
- Many solutions, which to choose?
- One that minimizes length of **b**, ||**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 estimate $\mathbf{X}^+$

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Singular Value Decomposition

- Any m by n matrix **X** can be factored into
  - $\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T$
  - **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

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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
```

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

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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 (the last diagonal element of **S**) appears to be zero!

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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!
  - ... e.g., so that $\mathbf{U}^{-1}=\mathbf{U}^T$
- How to form $\mathbf{S}^+$?
  - rank(**X**) =rank(**S**) and is the number of non-zero elements in **S**, rank(**X**) = r
  - Truncate the matrices to r columns
    - Same as setting elements in $\mathbf{S}^+$ to zero that correspond to zero elements in **S**

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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
```

```
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
```


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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 Ill-Conditioned Example

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

$$\mathbf{y} = \begin{bmatrix} 2 \\ 4 \\ 6 \\ 8 \end{bmatrix}$$

```
» 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
```


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The Solution is no Longer Sensitive to Minor Changes

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

b =
    0.4000
    0.8000
```

Inverse has been stabilized!

```
» y = [2 4 6.0001 8]';
» b = Xinv*y

b =
    0.4000
    0.8000
```


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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. **A**
- Collection of samples from GC-MS, or multiple batch runs

Algebra of Higher Order Tensors

- Higher order tensors are a natural way to store multiway data
    - analytical devices that produce a matrix per sample
    - batch process data
- Addition and scalar multiplication as expected
- Multiplication of tensors
    - definitions not universally accepted
    - need to be clear about the mathematical objective
        - kronecker, hadamard, …

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 $\leq \min(m,n)$ [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