Assignment 1

Part I

- phi/psi angles from PDB + secondary structure

Part II

- amino acid propensities

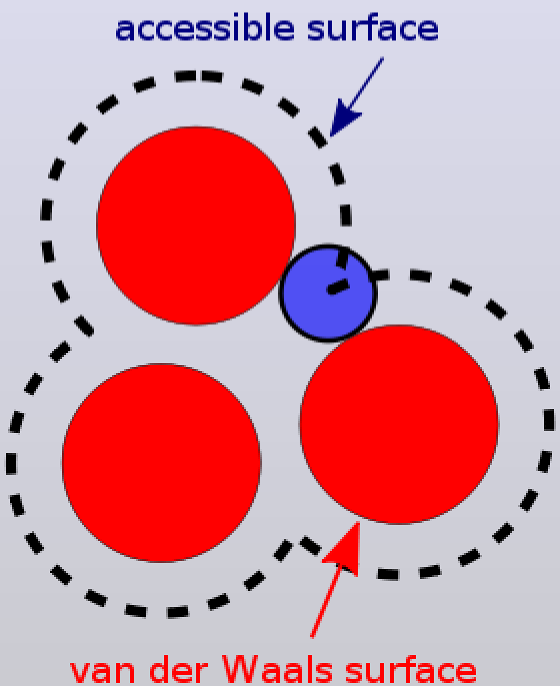
Part III

- interpretation & propose methods
- (read book)

If you have trouble start with part II, 1.1 is probably the most difficult question!

Surface Accessible area

Mathematically, one calculates the surface by integrating a step function f() over all points x on the surface of a sphere of radius r(atom) + r(water) around atom $\boldsymbol{i}$. f = 1 if a water sphere centered at x (by definition in contact with atom i) does not intersect with any other protein atom; otherwise f=0.

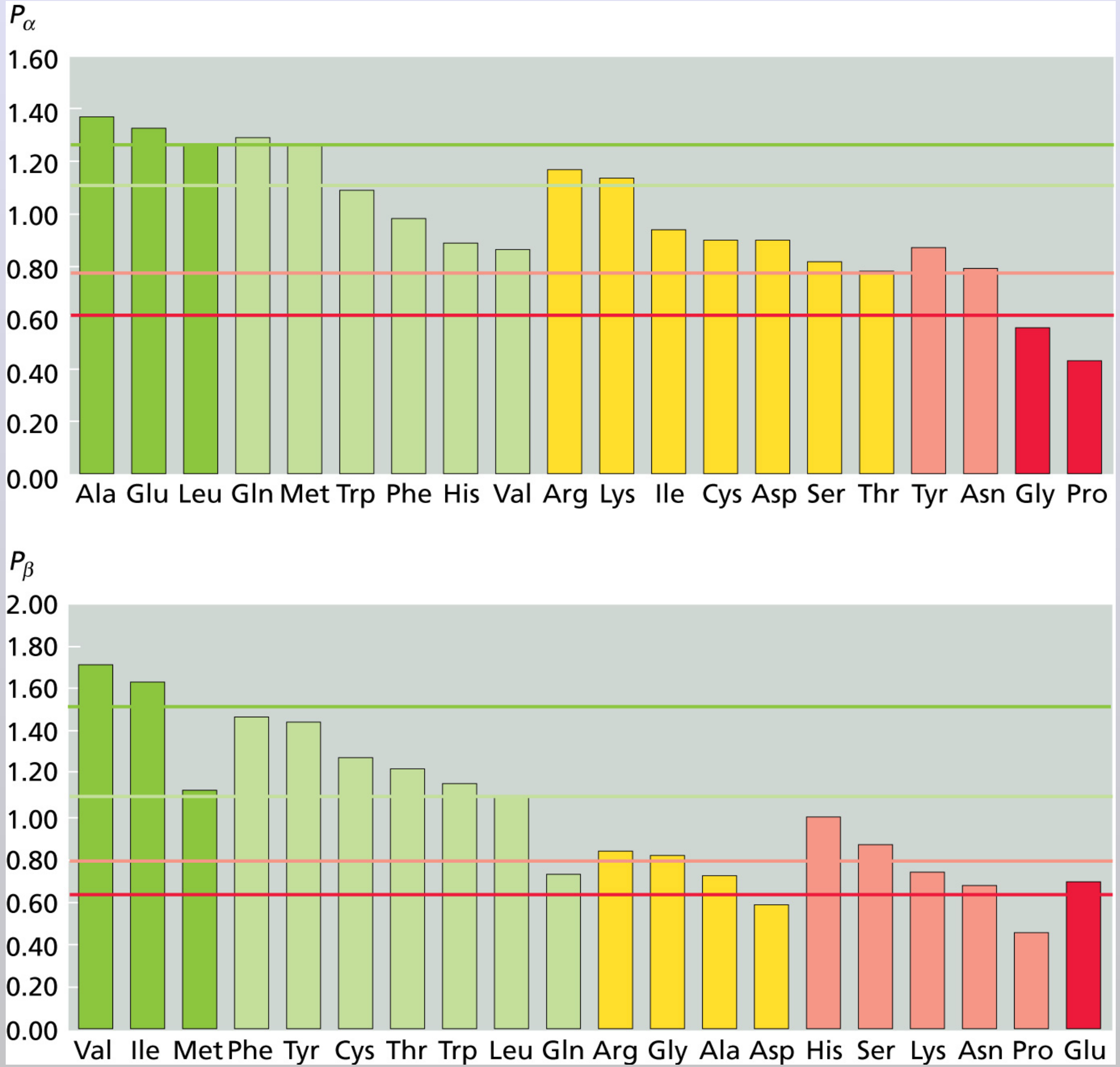


water molecules in contact with each residue:

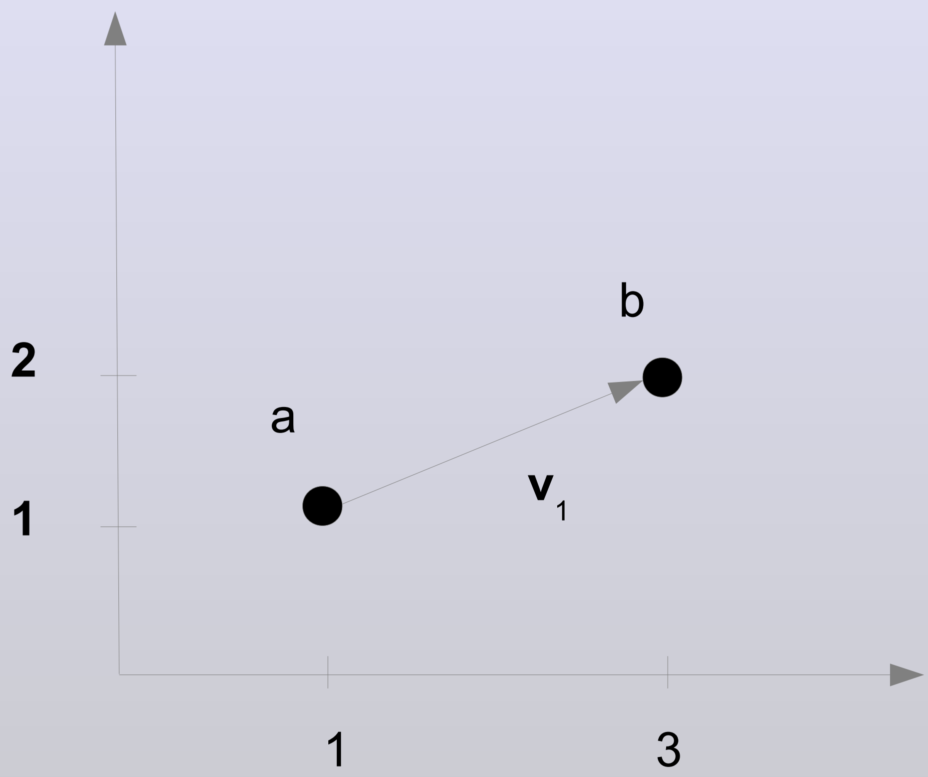
$$W = \frac{\text{Area}}{V(\text{water molecule})^{2/3}} \approx \frac{\text{Area}}{10}$$

Amino Acid propensities

$$P_{s,a} = \frac{f_{s,a}}{f_a}$$



Vectors - Recap

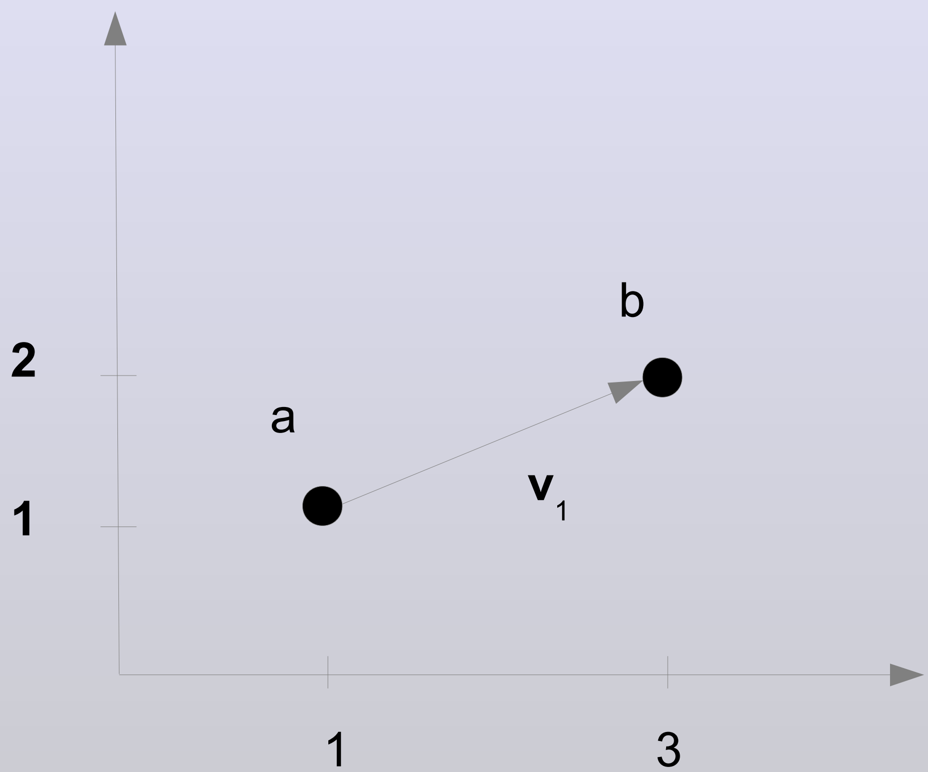


Points:
a = (1,1) =
b = (3,2)

Directional vector
$\mathbf{v}_1$ = **b** – **a**
= (,) – (,)
= (,)

a vector has a
- direction
- magnitude (length)

Vectors - Recap



a vector has a
- direction
- magnitude (length)

$\mathbf{v}_1 = (x,y)$

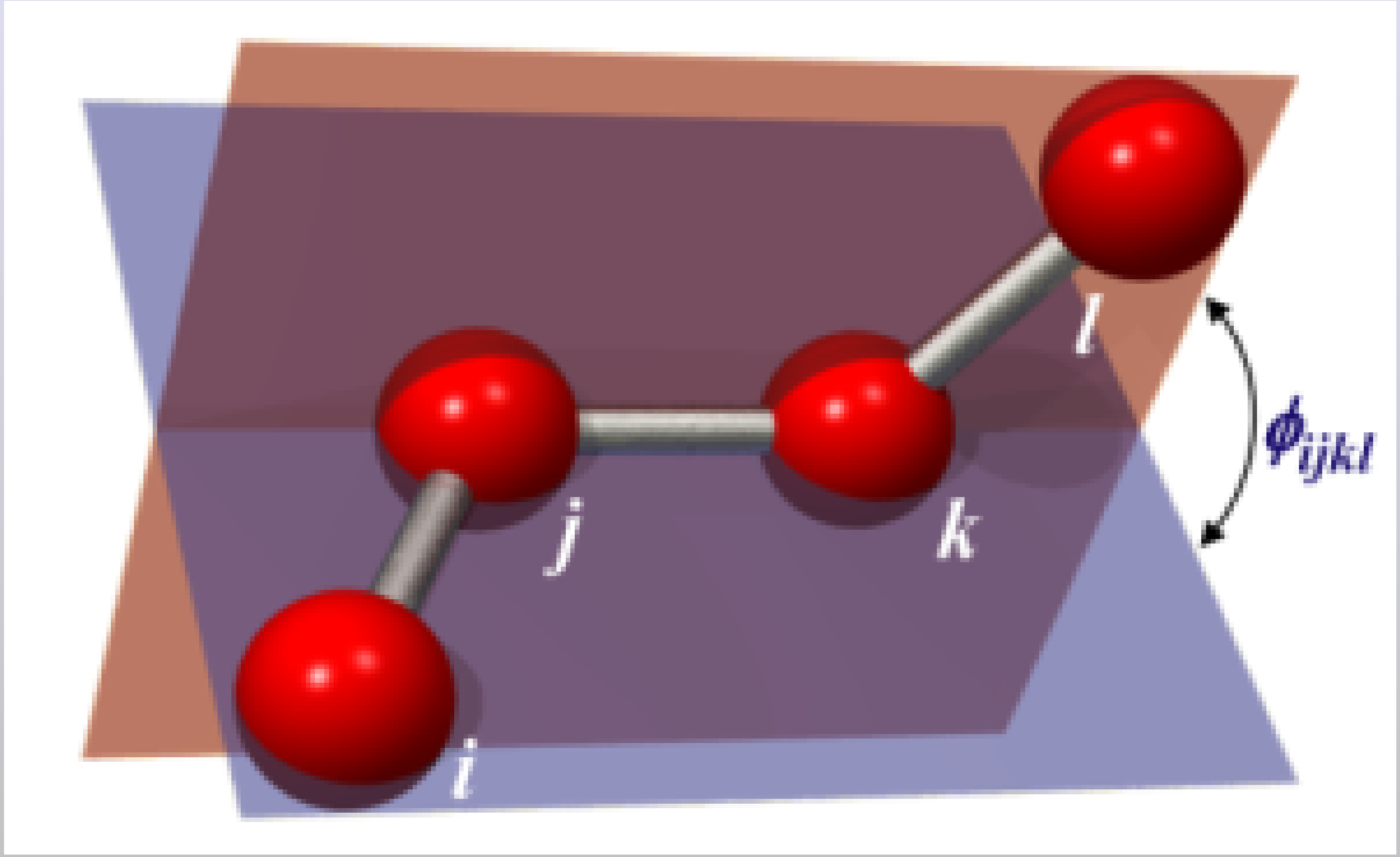
Magnitude vector:

$|\mathbf{v}_1| = \sqrt{x^2 + y^2}$

unit vector, vector of length 1

$$\mathbf{u}_1 = \frac{\mathbf{v}_1}{|\mathbf{v}_1|}$$

Torsion or Dihedral

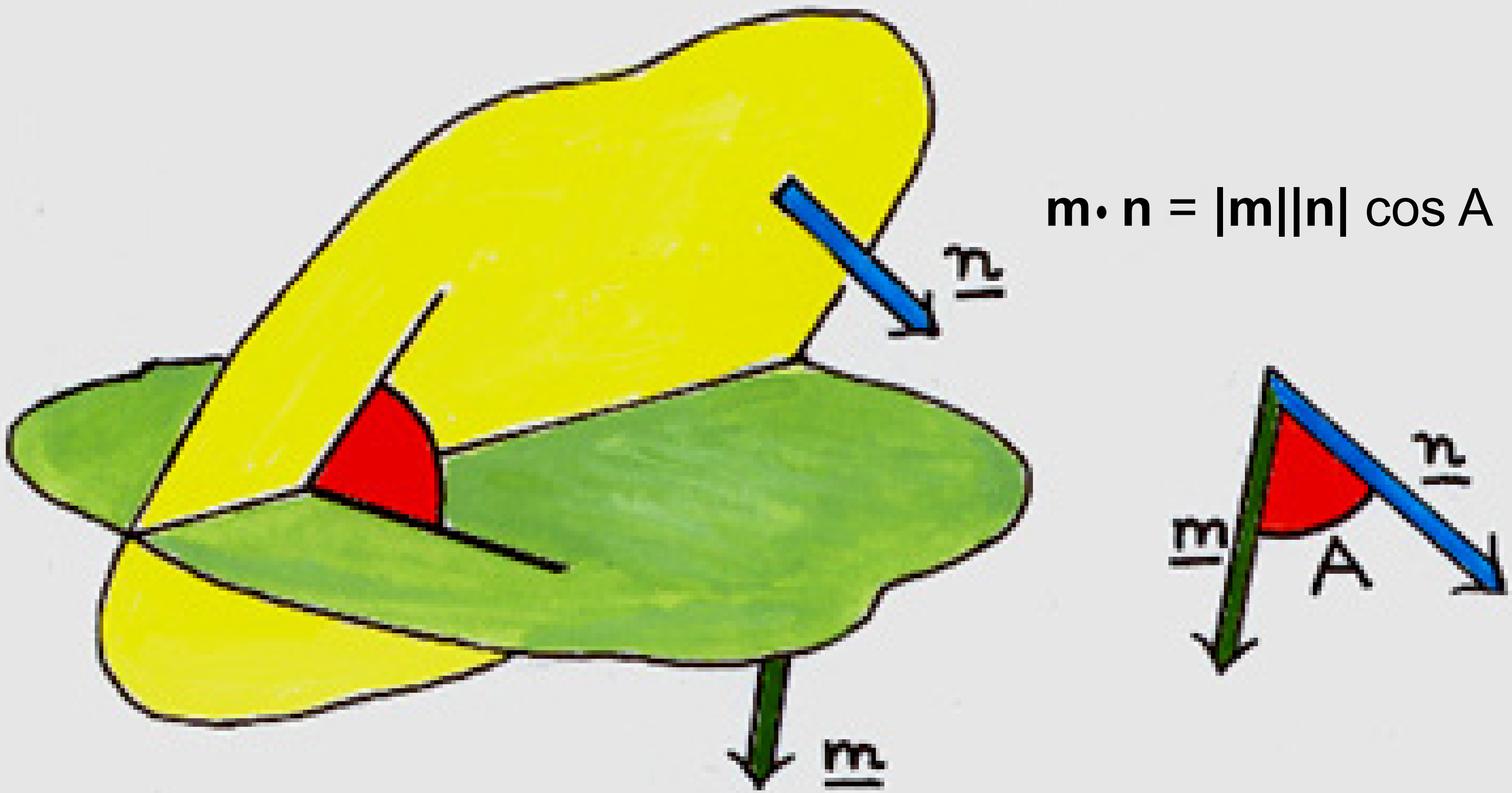


dot & cross product

$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \bullet \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} = a_x.b_x + a_y.b_y + a_z.b_z$$

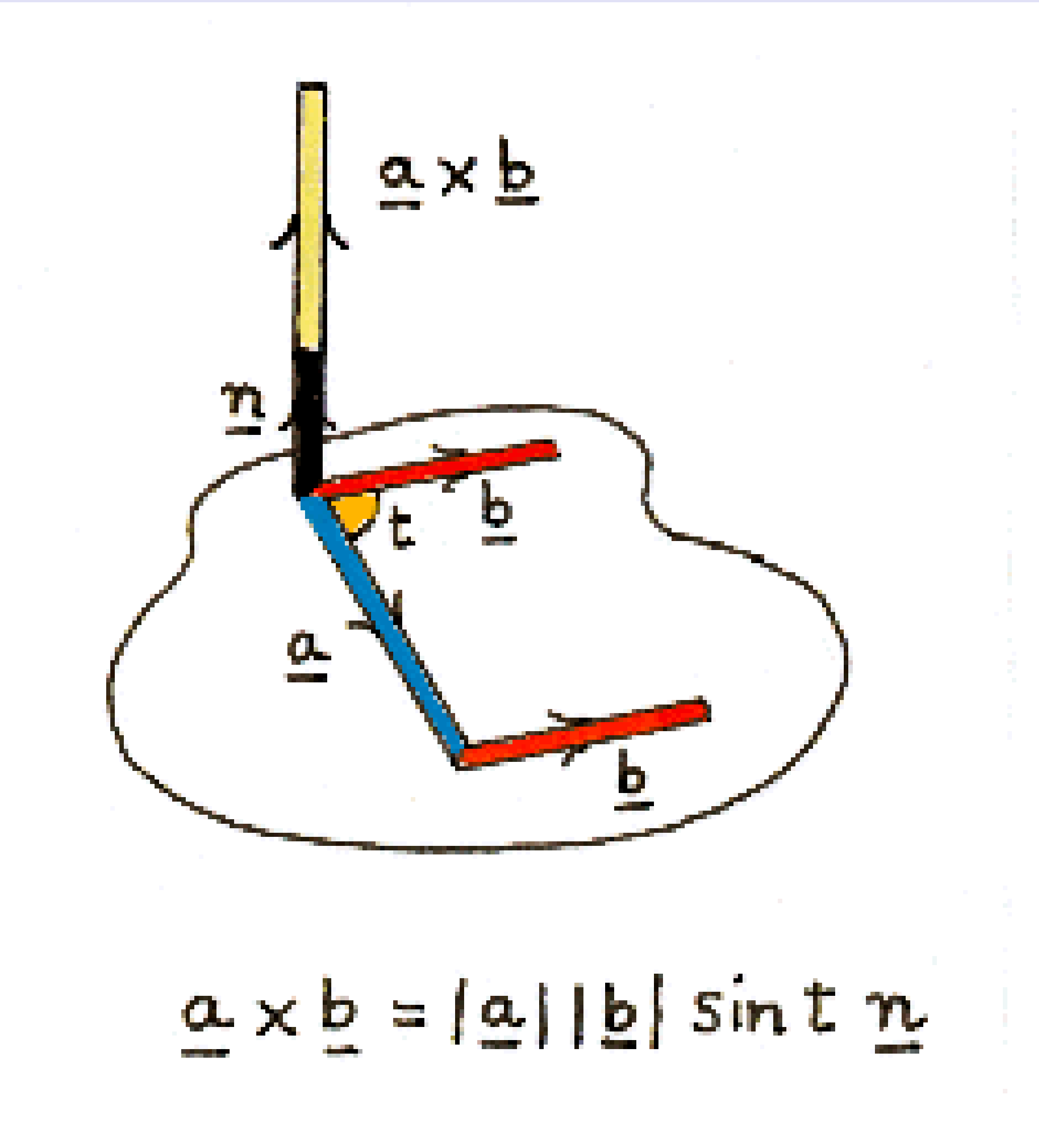
$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \times \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} = \begin{pmatrix} a_y b_z - b_y a_z \\ a_z b_x - b_z a_x \\ a_x b_y - b_x a_y \end{pmatrix}$$

Angles between planes



$\mathbf{m} \cdot \mathbf{n} = |\mathbf{m}||\mathbf{n}| \cos A$

cross product



The cross product will also give you a normal to the plane **a** and **b** lie in