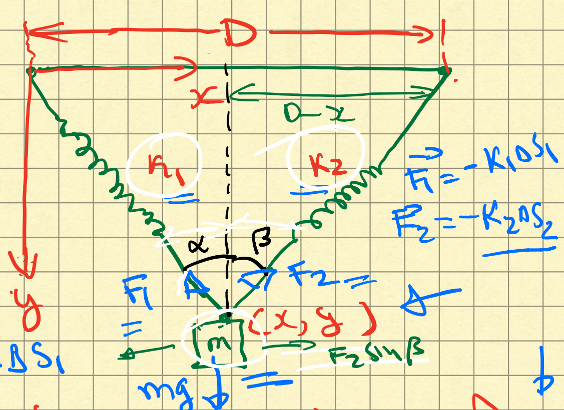
Today's Plan:

- So far we have discussed examples from
  - Scheduling (OR)
  - Resource allocation (Economics)

  Bazara, Sheralli & Shetty ✓
- Today, we will take up a couple of examples from physical sciences
  - Our examples revolve around minimization of potential energy.

Example: [Michael Heath, Scientific Computing: An Introductory Survey, Chapter-6 Ex 6.1]

- Spring-1 has length L_1 (unstretched) and spring constant K_1.
- Spring-2 has length L_2 and spring constant K_2.



Q] What is the equilibrium position of mass 'm' suspended from it?

$$\boxed{\vec{F_1} + \vec{F_2} + \vec{mg} = 0}$$

$F_1 \cos\alpha + F_2 \cos\beta = mg$

$F_1 \sin\alpha = F_2 \sin\beta$

Solution:

Let at the equilibrium position, coordinates of mass m be (x, y). Then,

$PE_1 = \frac{1}{2} K_1 \Delta S_1^2$

$PE_2 = \frac{1}{2} K_2 \Delta S_2^2$

- Elongation of spring-1 $= \sqrt{(x^2+y^2)} - L_1$
- Stretch in spring-2 $= \sqrt{(D-x)^2+y^2} - L_2$
- Total PE of the spring mass system

$$\boxed{V(x, y) = \frac{1}{2} K_1 \left(\sqrt{x^2+y^2} - L_1\right)^2 + \frac{1}{2} K_2 \left(\sqrt{(D-x)^2+y^2} - L_2\right)^2 - mgy}$$

$\Delta s_1 = \sqrt{x^2+y^2} - L_1 \qquad \Delta s_2 = \sqrt{(D-x)^2+y^2} - L_2$

$$\boxed{\min_{(x,y)} V(x,y) \quad \text{and} \quad (x^*, y^*) = \arg\min V(x,y)}$$

A minimum of an unconstrained minimization problem is always a stationary point.

$$\left.\frac{\partial V}{\partial x}\right|_{x^*} = 0 \Rightarrow K_1\left(\sqrt{x^2+y^2} - L_1\right)\frac{x}{\sqrt{x^2+y^2}} + K_2\left(\sqrt{(D-x)^2+y^2} - L_2\right)\frac{(D-x)(-1)}{\sqrt{(D-x)^2+y^2}} = 0$$

$$\Rightarrow K_1\left(\sqrt{x^2+y^2} - L_1\right)\sin\alpha = K_2\left(\sqrt{(D-x)^2+y^2} - L_2\right)\sin\beta$$

or $\quad F_1 \sin\alpha = F_2 \sin\beta$ Net Horizontal force is zero

Similary

$$\left.\frac{\partial V}{\partial y}\right|_{x^*} = 0 \quad K_1\left(\sqrt{x^2+y^2} - L_1\right)\frac{y}{\sqrt{x^2+y^2}} + K_2\left(\sqrt{(D-x)^2+y^2} - L_2\right)\frac{y}{\sqrt{(D-x)^2+y^2}} - mg = 0$$

or $K_1\left(\sqrt{x^2+y^2} - L_1\right)\cos\alpha + K_2\left(\sqrt{(D-x)^2+y^2} - L_2\right)\cos\beta = mg$

$$F_1\cos\alpha + F_2\cos\beta = mg.$$

From the fact that net force acting on mass m when at equilibrium, we get the same solution

$$\boxed{\begin{aligned} F_1 \sin\alpha &= F_2 \sin\beta \\ F_1 \sin\alpha + F_2 \cos\beta &= mg \end{aligned}}$$

where F_1 & F_2 are the restoring forces set in the two springs

An Example From Molecular Biology

Ref: J. Frederic Bonnans, J. Charles Gilbert, Claude Lemaréchal and Claudia A. Sagastizábal: Numerical Optimization: Theoritical and Practical Aspects.

Problem: Determine the geometry of a molecule (application in pharmacy, biochemistry)

- Experimental methods like x-ray, crystallography, nuclear magnetic resonance give you initial estimates
- Choice of method depends upon whether
  - chemical formula of the molecule is known
  - molecule is not available for experimentation
  - existing knowledge on its shape has to be refined.

Principle: The position of atoms in the space will be such that associated potential energy is minimum.

Let N be the number of atoms
e.g., 1000.

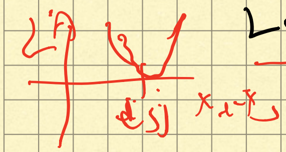
$x_i \in \mathbb{R}^3$ is the spatial position of ith atom.

Let $X = (x_1, x_2, \dots, x_N) \in \underline{\mathbb{R}^{3N}}$.

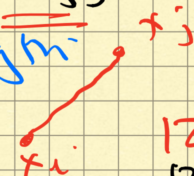
Let $f(X)$ → associates PE or conformational energy

$$f(X) = \sum_{i}\sum_{j}\left(L_{ij}(x_i, x_j) + V_{ij}(x_j, x_j)\right) + \sum_{i}\sum_{j}\sum_{k} A_{ijk}(x_i, x_j, x_k)$$

where Bond length component:



$$L_{ij}(x_i, x_j) = \lambda_{ij}\left(\underbrace{|x_i - x_j|}_{\text{Bond length}} - d_{ij}\right)^{2} \qquad \in \mathbb{R}^3$$



van der Waals energy

$$V_{ij}(x_i, x_j) = v_{ij}\left(\frac{\delta_{ij}}{|x_i - x_j|}\right)^{6} - \omega_{ij}\left(\frac{\delta_{ij}}{|x_i - x_j|}\right)^{12}$$

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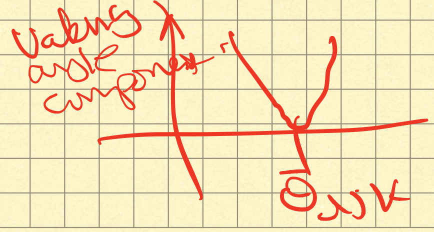
Here, the $\lambda_{ij}, v_{ij}, \omega_{ij}, \delta_{ij}$ are known constants depending upon pair of atoms involved (C–C, C–N etc)

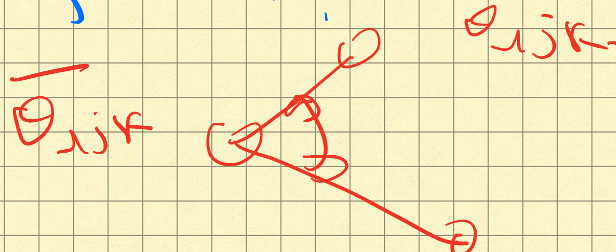
Valency angle component

$$A_{ijk}(x_i, x_j, x_k) = \alpha_{ijk}\left(\theta_{ijk} - \bar{\theta}_{ijk}\right)^{2}$$

where α_{ijk} and $\bar{\theta}_{ijk}$ are known constants

– Even galaxies seek minimum energy configuration!





$\min f(x)$