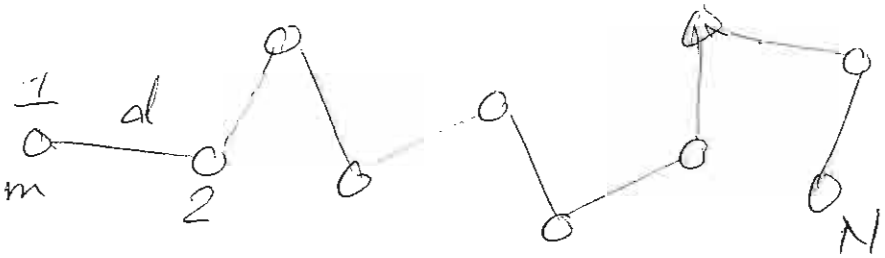
Constrained Variations

In mechanics we often have constraints that are active over whole periods of time, and so we have not just one or a few Lagrange multipliers, but a different multiplier at each instant of time, $\lambda(t)$!

Suppose we are interested in the motion of a polymer model comprising mass points joined by fixed-length bonds:

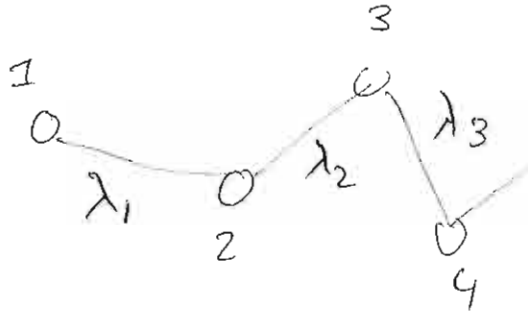


For simplicity, the masses all equal m and the bond distances are all d; there are no bond angle constraints.

One approach to this system is to build all the constraints into the definitions of the generalized coordinates — so no constraints are needed. With mass 1 specified by $\vec{r}_1$, we need two angles relative to $\vec{r}_1$ to specify $\vec{r}_2$, two more angles for $\vec{r}_3$, etc. for a total of $3 + 2(N-1) = 2N+1$ generalized coordinates. The resulting Lagrangian will be very complicated and will poorly reflect the symmetry of the system (angles close to 1 affect all the "downstream" points, but angles close to N have no affect on the

"upstream" points.).

An alternative approach is to use many Lagrange multipliers to impose the bond distance constraints:



The coordinates of the unconstrained mass points are just their cartesian coordinates $\vec{r}_1, \vec{r}_2, \ldots$ The constraint function associated with the first bond is

$$\left|\vec{r}_1(t) - \vec{r}_2(t)\right|^2 = d^2$$

to which we assign the multiplier $\lambda_1(t)$. Combining the Lagrangian

for unconstrained mass points with all the Lagrange multiplier terms we obtain the following functional:

$$F[\vec{r}_1(t), \ldots, \vec{r}_N(t)] = \int \Big[\tfrac{1}{2} m (\dot{\vec{r}}_1^{\,2} + \cdots + \dot{\vec{r}}_N^{\,2}) + \lambda_1(t) |\vec{r}_1 - \vec{r}_2|^2 + \cdots + \lambda_{N-1}(t) |\vec{r}_{N-1} - \vec{r}_N|^2 \Big] dt$$

This is much more symmetrical than what the minimal-generalized-coordinate approach produced. There is a small cost, in that the λ's need to be determined at each instant of time. But as the next few pages show, determining the λ's is a simple exercise in linear algebra.

Let's consider the case $N=2$:

$$\frac{\delta F}{\delta \vec{r}_1(t)} = -\frac{d}{dt}\left(m\dot{\vec{r}}_1\right) + \lambda_1(t)\,2(\vec{r}_1 - \vec{r}_2) = 0$$

$$\frac{\delta F}{\delta \vec{r}_2(t)} = -m\ddot{\vec{r}}_2 + 2\lambda_1(\vec{r}_2 - \vec{r}_1) = 0$$

$$\frac{2\lambda_1(t)}{m} = \lambda(t)$$

$$\ddot{\vec{r}}_1 = \lambda(\vec{r}_1 - \vec{r}_2) = -\ddot{\vec{r}}_2$$

The Lagrange multiplier is like a Hooke's law "constant", only it depends on time. A general approach for determining the λ's starts by taking time derivatives of the constraint equations:

$$\frac{d^2}{dt^2}\left[(\vec{r}_1 - \vec{r}_2)\cdot(\vec{r}_1 - \vec{r}_2)\right] = 0$$

$$\Rightarrow (\ddot{\vec{r}}_1 - \ddot{\vec{r}}_2) \cdot (\vec{r}_1 - \vec{r}_2) + |\dot{\vec{r}}_1 - \dot{\vec{r}}_2|^2 = 0$$

Substituting the accelerations from the equations of motion,

$$2\lambda |\vec{r}_1 - \vec{r}_2|^2 + |\dot{\vec{r}}_1 - \dot{\vec{r}}_2|^2 = 0$$

$$\Rightarrow \lambda = -\frac{1}{2} \frac{|\dot{\vec{r}}_1 - \dot{\vec{r}}_2|^2}{d^2}$$

The equations of motion may now be solved with this time-dependent λ:

$$\ddot{\vec{r}}_1 = -\frac{1}{2} \frac{|\dot{\vec{r}}_1 - \dot{\vec{r}}_2|^2}{d^2} (\vec{r}_1 - \vec{r}_2) = -\ddot{\vec{r}}_2$$

You can check that this is the correct central acceleration of two points in a circular orbits about the bond-center.

When the polymer has N mass points and $N-1$ bonds, a system of linear equations involving $N-1$ λ's has to be solved at each instant of time.