The Maud[¶] Algorithm

Potential between points

We are looking for stationary values (minima, maxima, saddle points etc.) of the following potential between a number of points in 2 or 3 dimensional space:

Consider two typical points with position vectors $\mathbf{r}_i$ and $\mathbf{r}_j$. The contribution to the potential from these two points, P_{ij}, is a function only of their separation L_{ij} which can obtained from $L_{ij}^2 = \left(\mathbf{r}_i - \mathbf{r}_j\right) \bullet \left(\mathbf{r}_i - \mathbf{r}_j\right)$.

All points repel each other with an 'inverse square' potential $P_{ij} = \dfrac{a^3 Q}{L_{ij}}$ where Q (which has the units of force over length) and a (which is a length) are constants. In addition some points are tied together with 'linear zero unstressed length springs' which have an **additional** contribution to the potential of $\dfrac{QL_{ij}^2}{2}$. Thus

The total potential is $P = \sum_i \sum_j P_{ij}$ where $i \neq j$ in the summation.

For equilibrium, that is stationary values of the potential, we require the 'out of balance forces', $\mathbf{F}_m = \dfrac{\partial P}{\partial \mathbf{r}_m} = \sum_i \sum_j \dfrac{\partial P_{ij}}{\partial \mathbf{r}_m} = 0$ for all m.

The 'stiffness matrix', $\mathbf{K}$ has elements $\mathbf{K}_{mn} = \dfrac{\partial^2 P}{\partial \mathbf{r}_m \partial \mathbf{r}_n} = \sum_i \sum_j \dfrac{\partial^2 P_{ij}}{\partial \mathbf{r}_m \partial \mathbf{r}_n}$. Note that $\mathbf{K}_{mn}$ is a symmetric second order tensor, or if one prefers 2 by 2 matrix in 2 dimensions or a 3 by 3 matrix in 3 dimensions. $\mathbf{K}$ is a much larger square matrix who size is determined by the number of points. Note that we will not need to compute $\mathbf{K}$.

The partial derivative $\dfrac{\partial P_{ij}}{\partial \mathbf{r}_m} = 0$ if $m \neq i$ and $m \neq j$ and

$$
\begin{aligned}
\frac{\partial P_{ij}}{\partial \mathbf{r}_i} = -\frac{\partial P_{ij}}{\partial \mathbf{r}_j} = \frac{dP_{ij}}{dL_{ij}} \frac{\partial L_{ij}}{\partial \mathbf{r}_i} &= \frac{dP_{ij}}{dL_{ij}} \frac{\partial}{\partial \mathbf{r}_i} \sqrt{\left(\mathbf{r}_i - \mathbf{r}_j\right) \bullet \left(\mathbf{r}_i - \mathbf{r}_j\right)} \\
&= \frac{dP_{ij}}{dL_{ij}} \frac{2\left(\mathbf{r}_i - \mathbf{r}_j\right)}{2\sqrt{\left(\mathbf{r}_i - \mathbf{r}_j\right) \bullet \left(\mathbf{r}_i - \mathbf{r}_j\right)}} = \frac{dP_{ij}}{dL_{ij}} \frac{\left(\mathbf{r}_i - \mathbf{r}_j\right)}{L_{ij}} = \frac{T_{ij}}{L_{ij}} \left(\mathbf{r}_i - \mathbf{r}_j\right)
\end{aligned}.
$$

[¶] After the film *Ma nuit chez Maud* by Éric Rohmer.

where $T_{ij} = \frac{dP_{ij}}{dL_{ij}}$ is the 'tension' and $\frac{T_{ij}}{L_{ij}}$ is the 'tension coefficient'.

$$\frac{\partial^2 P_{ij}}{\partial \mathbf{r}_i^2} = \frac{\partial^2 P_{ij}}{\partial \mathbf{r}_j^2} = -\frac{\partial^2 P_{ij}}{\partial \mathbf{r}_i \partial \mathbf{r}_j} = \frac{d^2 P_{ij}}{dL_{ij}^2}\frac{\partial L_{ij}}{\partial \mathbf{r}_i}\frac{(\mathbf{r}_i - \mathbf{r}_j)}{L_{ij}} + \frac{dP_{ij}}{dL_{ij}}\frac{\mathbf{I}}{L_{ij}} - \frac{dP_{ij}}{dL_{ij}}\frac{\partial L_{ij}}{\partial \mathbf{r}_i}\frac{(\mathbf{r}_i - \mathbf{r}_j)}{L_{ij}^2}$$

$$= \frac{dP_{ij}}{dL_{ij}}\frac{\mathbf{I}}{L_{ij}} + \left(\frac{d^2 P_{ij}}{dL_{ij}^2} - \frac{1}{L_{ij}}\frac{dP_{ij}}{dL_{ij}}\right)\frac{(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{r}_i - \mathbf{r}_j)}{L_{ij}^2} = \frac{T_{ij}}{L_{ij}}\mathbf{I} + \left(\frac{dT_{ij}}{dL_{ij}} - \frac{T_{ij}}{L_{ij}}\right)\frac{(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{r}_i - \mathbf{r}_j)}{L_{ij}^2}$$

$\mathbf{I}$ is the unit second order tensor. $\frac{dT_{ij}}{dL_{ij}}\frac{(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{r}_i - \mathbf{r}_j)}{L_{ij}^2}$ is the elastic stiffness and $\frac{T_{ij}}{L_{ij}}\left(\mathbf{I} - \frac{(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{r}_i - \mathbf{r}_j)}{L_{ij}^2}\right)$ is the geometric stiffness.

The algorithm

i. Calculate the out of balance forces, $\mathbf{F}_m = \frac{\partial P}{\partial \mathbf{r}_m} = \sum_i \sum_j \frac{\partial P_{ij}}{\partial \mathbf{r}_m}$

ii. Move the nodes in a direction to try and reduce $\mathbf{F}_m$. The 'tensor' approach moves a typical node by an amount $\delta\mathbf{r}_m$ to satisfy $\delta\mathbf{r}_m \bullet \mathbf{K}_{mm} = \gamma\mathbf{F}_m$ in which there is no summation on the subscript. Thus each node is moved taking into account only the out of balance force experienced by the node itself and the stiffness experienced at the node if all the other nodes are fixed. Thus $\delta\mathbf{r}_m = \gamma\mathbf{F}_m \bullet \mathbf{K}_{mm}^{-1}$. Note that the repulsive forces may mean that some of the principal values of $\mathbf{K}_{mm}$ are positive. The value of γ is chosen as a compromise between speed and stability. The 'scalar' approach is similar except the formula $\delta\mathbf{r}_m = \frac{\gamma\mathbf{F}_m}{\mathrm{Tr}(\mathbf{K}_{mm})}$ is used. The trace, $\mathrm{Tr}(\mathbf{K}_{mm})$ is the sum of principal values of $\mathbf{K}_{mm}$, which is probably always positive.

iii. Go back to i.

The process is speeded up using Alistair Day's 'dynamic relaxation' technique†, which carries over the 'velocity' of the nodes from the previous cycle, with some damping.

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† A.S.Day, *An introduction to dynamic relaxation*. The Engineer **219**,219-221(1965).