0.1 Eigenvalues

In this document we derive the eigenvalues of the Rouse matrix. The Rouse matrix defines the connection in the harmonic potential of the Rouse polymer. The system of differential equation governing the dynamics of the chain comprised of N monomers is

$$\frac{d[X(t)]}{dt} = -k[R][X(t)] + [g(t)] \tag{1}$$

where the [.] notation represents a matrix (vector), $[g(t)]$ is an N by 1 vector of normally distributed numbers with mean 0 and STD =1, k is a constant and the matrix $[R]$ is defined as:

$$R = \begin{bmatrix} 1 & -1 & 0 & 0 & ... & & 0 \\ -1 & 2 & -1 & 0 & ... & & 0 \\ 0 & -1 & 2 & -1 & ... & & 0 \\ . & & & . & & & . \\ . & & & . & & & . \\ 0 & & & & -1 & 2 & -1 \\ 0 & & & & 0 & -1 & 1 \end{bmatrix} \tag{2}$$

To find the eigenvalues we calculate

$$D_N = |[R] - \lambda[I]| = 0$$

which gives us a matrix of the form

$$R = \begin{bmatrix} y & -1 & 0 & 0 & ... & & 0 \\ -1 & x & -1 & 0 & ... & & 0 \\ 0 & -1 & x & -1 & ... & & 0 \\ . & & & . & & & . \\ . & & & . & & & . \\ 0 & & & & -1 & x & -1 \\ 0 & & & & 0 & -1 & y \end{bmatrix}$$

with $x = 2 - \lambda$, and $y = x - 1$.

Developing the determinant by the last column we find a recursion relation as follows

$$D_N = yD_{N-1} - D_{N-2} \tag{3}$$

since the recursion relation is slightly different for D_{N-1}, bt remains the same for all $j \leq N-1$, we solve the recursion relation for D_{N-1} and then return to define the last term D_N using the relation above.

The recurrence relation is:

$$D_z = xD_{z-1} - Dz - 2$$

with the boundary conditions

$$D_1 = y$$

$$D_2 = xy - 1$$

We note that according to the Rouse matrix $x = y + 1$.

The particular solution to the recursion relation is

$$D_z = e^{iz\theta} \tag{4}$$

substituting it into the recursion relation gives

$$e^{iz\theta} = xe^{i(z-1)\theta} - e^{i(z-2)\theta} \tag{5}$$

hence

$$x = 2cos(\theta) \tag{6}$$

The general solution can then be defined as

$$D_z = Ae^{iz\theta} + Be^{-iz\theta}$$

where A and B are some constants to be defined.

Using the boundary conditions we get

$$y = Ae^{i\theta} + Be^{-i\theta}$$

$$A = \frac{y - Be^{-i\theta}}{e^{i\theta}} = (2\cos(\theta) - 1)e^{-i\theta} - Be^{-2i\theta} = \frac{1 - e^{i\theta}}{e^{-i\theta} - e^{i\theta}} = e^{i\theta/2}\frac{e^{-i\theta/2} - e^{i\theta/2}}{-2i\sin(\theta)} = \frac{e^{i\theta/2}}{2\cos(\theta/2)}$$

and

$$B = \frac{e^{-i\theta} - 1}{e^{-i\theta} - e^{i\theta}} = \frac{e^{-i\theta/2}}{2cos(\theta/2)}$$

The general solution is now

$$D_z = \frac{e^{i\theta/2}}{2\cos(\theta/2)}e^{iz\theta} + \frac{e^{-i\theta/2}}{2\cos(\theta/2)}e^{-iz\theta} = \frac{\cos((z+1/2)\theta)}{\cos(\theta/2)} \tag{7}$$

Since the determinant must vanish, we have

$$D_N = yD_{N-1} - D_{N-2} = 0$$

substituting the expressions for D_{N-1} and D_{N-2} into the equation above yields

$$yD_{N-1} - D_{N-2} = D_1 D_{N-1} - D_{N-2} =$$
$$\frac{\cos(3\theta/2)}{\cos(\theta/2)} \frac{\cos((N-1/2)\theta)}{\cos(\theta/2)} - \frac{\cos((N-3/2)\theta)}{\cos(\theta/2)} = 0$$

therefore

$$\cos(3\theta/2)\cos((N-1/2)\theta) = \cos((N-3/2)\theta)\cos(\theta/2)$$

displaying the trigonometric functions as sum of exponentials we can get

$$\cos((N+1)\theta) - \cos((N-1)\theta) = 0$$

which gives

$$-2\sin(N\theta)\sin(\theta) = 0$$

therefore

$$\theta = \frac{p\pi}{N}$$

$p = 0, 1..., N-1$ (since we have N solutions)

The eigenvalues are then

$$\lambda_p = 2 - x = 2 - 2\cos(\theta_p) = 2\left(1 - \cos(\frac{p\pi}{N})\right) = 4\sin^2(\frac{p\pi}{2N}) \tag{8}$$

$p = 0, 1, ..., (N-1)$

0.2 Eigenvectors

the k^{th} entry in the p^{th} eigenvector is

$$c_k = \sqrt{\frac{2}{N}}\sin(\frac{k\pi p}{N}) \tag{9}$$

with $k = 1, 2, .., N$ and $p = 0, 1, ...N-1$