0.1 Eigenvalues of the Rouse Matrix

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

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

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:

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

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

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

substituting it into the recursion relation gives

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

hence

$$x = 2cos(\theta)$$

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

$$D_z = \frac{e^{i\theta/2}}{2\cos(\theta/2)}e^{iz\theta} + \frac{e^{-i\theta/2}}{2\cos(\theta/2)}e^{-iz\theta} = \frac{\cos((z+1/2)\theta)}{\cos(\theta/2)} \tag{3}$$

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

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

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

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

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

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

0.3 Eigenvalues of the Rouse Ring

Connecting bead 1 and N to form a ring, we now search for the eigenvalues of the new *Rouse ring* matrix, R, harboring such a connection. For this end, we have to calculate the determinant of the matrix

$$D_N = |R - \lambda I| = \begin{vmatrix} x & -1 & 0 & 0 & \ldots & & & -1 \\ -1 & x & -1 & 0 & \ldots & & & 0 \\ 0 & -1 & x & -1 & \ldots & & & 0 \\ . & & & . & & & & . \\ . & . & & & . & & & \\ . & & & -1 & x & -1 & & 0 \\ 0 & & & & -1 & x & & -1 \\ -1 & . & . & . & 0 & -1 & & x \end{vmatrix}_{N\times N}$$

with $x = 2 - \lambda$. We can apply to the matrix of size $(N-1)\times(N-1)$ the same procedure as before and try to solve it recursively. The boundary conditions now read

$$D_1 = x; D_2 = x^2 - 1$$

According to the solution in section 0.1 and in [1], we have

$$D_{N-1} = \frac{\sin(N\theta)}{\sin(\theta)}$$

The relationship between D_N and D_{N-1} is found by developing the determinant of D_N according to the last column

$$D_N = x(-1)^{2N}D_{N-1} + (-1)(-1)^{2N-1}D^* + (-1)(-1)^{N+1}D^{**} = xD_{N-1} + D^* + (-1)^{N+2}D^{**}$$

with the determinant D^* and D^{**} defined as the minors

$$D^* = \begin{vmatrix} x & -1 & 0 & 0 & \ldots & 0 \\ -1 & x & -1 & 0 & \ldots & 0 \\ 0 & -1 & x & -1 & \ldots & \\ . & & & . & & \\ . & & & . & & \\ . & & & -1 & x & -1 \\ -1 & & & & 0 & -1 \end{vmatrix}_{(N-1)\times(N-1)} \qquad D^{**} = \begin{vmatrix} -1 & x & -1 & 0 & \ldots & 0 \\ 0 & -1 & x & -1 & \ldots & 0 \\ . & & & . & & . \\ . & & & . & & . \\ . & & & -1 & x & -1 \\ 0 & & & & -1 & x \\ -1 & & & & 0 & -1 \end{vmatrix}_{(N-1)\times(N-1)}$$

We calculate the determinants D^* and D^{**} by minors according to the last row to get

$$D^* = (-1)(-1)^{2N-2}D_{N-2} + (-1)(-1)^{N-1+1}(-1)^{N-2} = (-1)^{2N-1}[D_{N-2}+1]$$

$$D^{**} = (-1)(-1)^{2N-2}(-1)^{N-2}+(-1)(-1)^{1+N-1}D_{N-2} = (-1)^{3N-3}+(-1)^{N+1}D_{N-2}$$

Therefore,

$$\begin{aligned}
D_N &= xD_{N-1} + (-1)^{2N-1}[D_{N-2}+1] + (-1)^{N+2}[(-1)^{3N-3} + (-1)^{N+1}D_{N-2}] \\
&= xD_{N-1} + (-1)^{2N-1}[D_{N-2}+1] + (-1)^{4N-1} + (-1)^{2N+3}D_{N-2} \\
&= xD_{N-1} + D_{N-2}[(-1)^{2N-1} + (-1)^{2N+3}] + (-1)^{2N-1} + (-1)^{4N-1} \\
&= xD_{N-1} - 2D_{N-2} - 2
\end{aligned}$$

Substituting the solution for D_{N-1} and D_{N-2}, we get

$$D_N = \frac{x\sin(N\theta) - 2\sin((N-1)\theta) - 2\sin(\theta)}{\sin(\theta)} = 0$$

Further simplification of D_N leads to

$$\begin{aligned}
D_N &= 2\frac{\cos(\theta)\sin(N\theta) - [\sin((N-1)\theta) + \sin(\theta)]}{\sin(\theta)} \\
&= \frac{2}{\sin(\theta)}[\cos(\theta)\sin(N\theta) - [2\sin(\frac{N\theta}{2})\cos(\frac{(N-2)\theta}{2})] \\
&= \frac{4}{\sin(\theta)}[\cos(\theta)\sin(\frac{N\theta}{2})\cos(\frac{N\theta}{2}) - \sin(\frac{N\theta}{2})[\cos(\frac{N\theta}{2})\cos(\theta) + \sin(\frac{N\theta}{2})\sin(\theta)] \\
&= -4\sin^2(\frac{N\theta}{2})
\end{aligned}$$

Equating $D_N = 0$ we get the solutions

$$\theta_p = \frac{2\pi p}{N}$$

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

Therefore, the eigenvalues of the Rouse ring are

$$\lambda_p = 2(1 - cos(\theta_p)) = 2(1 - cos(2\pi p/N))$$

Since $\cos(\frac{2\pi\phi}{N}) = \cos(\frac{2\pi(N-\phi)}{N})$, we have eigenvalues multiplicities. In our case, setting $\phi = p$ we have $\cos(\frac{2\pi p}{N}) = \cos(\frac{2\pi(N-p)}{N})$ for $p = 1, 2, 3, .., (N-2)$. For the end-values, $p = 0$ and $p = N-1$ the eigenvalues are unique.

0.4 Eigenvectors of the Rouse Ring

0.4.1 eigenvalues with multiplicity 1

The eigenvectors corresponding to eigenvalues with algebraic multiplicity 1. From the relation $Rv = \lambda v$ where v is an eigenvector. We have the recursion relation for the component of the v vector, $j = 2, ..., N-1$

$$v_j = \frac{v_{j-1} + v_{j+1}}{2\cos(\theta)}$$

The boundary conditions are

$$v_1 = \frac{v_2 + v_N}{2\cos(\theta)}, \quad v_N = \frac{v_1 + v_{N-1}}{2\cos(\theta)}$$

Rearranging the terms for v_1 and v_N

$$v_1 = \frac{2v_2\cos(\theta) + v_{N-1}}{4\cos^2(\theta) - 1} \qquad v_N = \frac{v_2 + 2v_{N-1}\cos(\theta)}{4\cos^2(\theta) - 1}$$

where, again, we have used the relation $2 - \lambda = 2\cos(\theta)$, resulting from substituting the particular solution $v_j = e^{ij\theta}$ into the recursion relation for v_j.

Substituting the general solution into the first boundary condition we get

$$A(e^{i\theta}(4\cos^2(\theta)-1)-2\cos(\theta)e^{2i\theta}-e^{i(N-1)\theta}) = -B(e^{-i\theta}(4\cos^2(\theta)-1)-2\cos(\theta)e^{-2i\theta}-e^{-i(N-1)\theta})$$

if we set

$$f(\theta) = (e^{i\theta}(4\cos^2(\theta) - 1) - 2\cos(\theta)e^{2i\theta} - e^{i(N-1)\theta})$$

then

$$Af(\theta) = -Bf(-\theta)$$

notice that

$$f(\theta) = \left\langle [4\cos^2(\theta) - 1, 2\cos(\theta), 1], -[e^{i\theta}, e^{2i\theta}, 1] \right\rangle$$

and

$$f(-\theta) = \left\langle [4\cos^2(\theta) - 1, 2\cos(\theta), 1], -[e^{-i\theta}, e^{-2i\theta}, 1] \right\rangle$$

The vectors $[e^{-i\theta}, e^{-2i\theta}, 1]$ and $[e^{i\theta}, e^{2i\theta}, 1]$ are opposite in directions but otherwise equal. Indeed

$$cos(\phi) = \frac{\left\langle [e^{-i\theta}, e^{-2i\theta}, 1], [e^{i\theta}, e^{2i\theta}, 1] \right\rangle}{\sqrt{3}\sqrt{3}} = \frac{3}{\sqrt{3}\sqrt{3}} \Rightarrow \phi = k\pi \qquad k = 0, 1, 2, ...$$

with ϕ the angle between vectors. Hence, we conclude $f(\theta) = -f(-\theta)$ and therefore

$$A = B$$

and the general solution becomes

$$v_j = A(e^{ij\theta} + e^{-ij\theta}) = 2A\cos(j\theta)$$

The values of v_1 and v_N can be written as

$$v_1 = \frac{2A[2\cos(2\theta)\cos(\theta) + \cos((N-1)\theta)]}{4\cos^2(\theta) - 1} \qquad v_N = \frac{2A[\cos(2\theta) + 2\cos(\theta)\cos((N-1)\theta)]}{4\cos^2(\theta) - 1}$$

Using the normalization conditions, namely $\sum_{j=1}^{N} v_j^2 = 1$, we write

$$\sum_{j=2}^{N-1} A^2\cos^2(j\theta) + v_1^2 + v_N^2 = 1$$

and therefore

$$\begin{aligned} A &= (\sum_{j=2}^{N-1}\cos^2(j\theta) + \left(\frac{2[2\cos(2\theta)\cos(\theta) + \cos((N-1)\theta)]}{4\cos^2(\theta) - 1}\right)^2 \\ &+ \left(\frac{2[\cos(2\theta) + 2\cos(\theta)\cos((N-1)\theta)]}{4\cos^2(\theta) - 1}\right)^2)^{-0.5} \end{aligned}$$

0.4.2 eigenvectors with multiplicity 2

Bibliography

[1] Y-H Lin. *Polymer Viscoelasticity: Basics, Molecular Theories, Experiments and Simulations*. World Scientific, 2011.