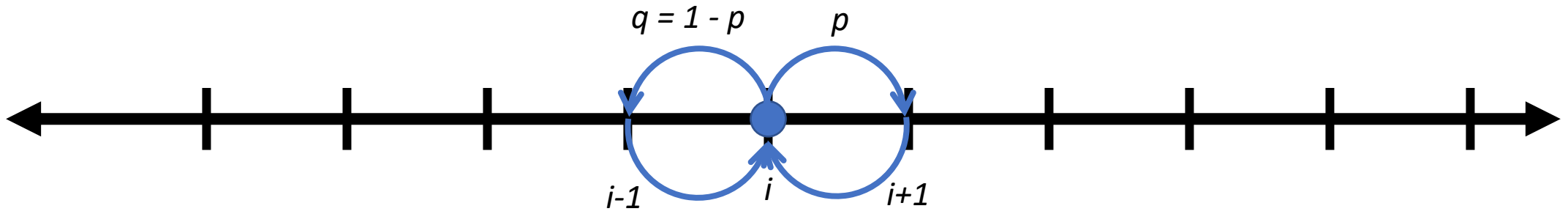
1D random walk

```
p ← value
for each molecule do rand = random(100)
    if rand ≤ p then
        go right
    else
        go left
    end if
end for
```



For a system with equal diffusivity in all directions, q = p

$$\frac{dn_i}{dt} = pn_{i-1} + pn_{i+1} - 2pn_i$$

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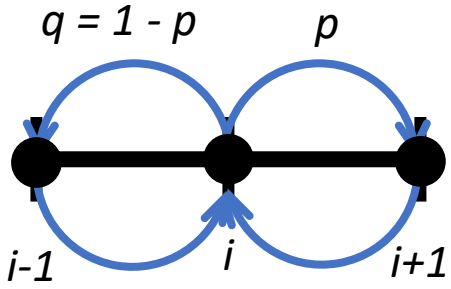


For a system with equal diffusivity in all directions, q = p

$$\frac{dn_{i-1}}{dt} = pn_i - pn_{i-1}$$

$$\frac{dn_i}{dt} = pn_{i-1} + pn_{i+1} - 2pn_i$$

$$\frac{dn_{i+1}}{dt} = pn_i - pn_{i+1}$$

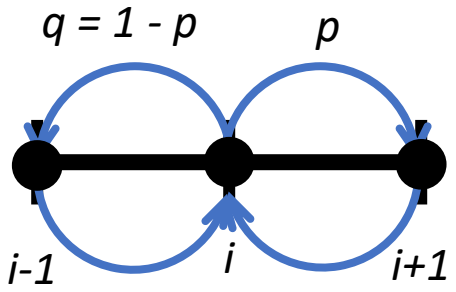
$$\begin{bmatrix} \dot{n}_{i-1} \\ \dot{n}_i \\ \dot{n}_{i+1} \end{bmatrix} = \begin{bmatrix} -p & p & 0 \\ p & -2 & p \\ 0 & p & -p \end{bmatrix} \begin{bmatrix} n_{i-1} \\ n_i \\ n_{i+1} \end{bmatrix}$$

$$\dot{n}(t) = A(t)n(t)$$

$$\mathbf{A\,n = \lambda\,n}$$

$$\mathbf{n(t)} = \sum_{k=1}^{N} c_k n_k e^{\lambda_k t}$$

1D random walk



$$\begin{bmatrix} \dot{n}_{i-1} \\ \dot{n}_i \\ \dot{n}_{i+1} \end{bmatrix} = \begin{bmatrix} -p & p & 0 \\ p & -2 & p \\ 0 & p & -p \end{bmatrix} \begin{bmatrix} n_{i-1} \\ n_i \\ n_{i+1} \end{bmatrix}$$

$$\dot{n}(t) = A(t)n(t)$$

Eigenmode solution

$$\mathbf{n(t)} = \sum_{k=1}^{N} c_k n_k e^{\lambda_k t}$$

Eigenvalue equations

$$\det(\mathbf{A} - \lambda_k \mathbf{I})\mathbf{v} = 0$$

Eigendecomposition

$$\mathbf{Av} = \lambda\mathbf{v}$$

$$\mathbf{AQ} = \mathbf{Q\Lambda}$$

$$\mathbf{A} = \mathbf{Q\Lambda Q^{-1}}$$

Finding the **eigenvalues**

$$\mathbf{A} - \lambda_k \mathbf{I} = \begin{bmatrix} -p - \lambda & p & 0 \\ p & -2 - \lambda & p \\ 0 & p & -p - \lambda \end{bmatrix}$$

$$\begin{aligned} \det(\mathbf{A} - \lambda_k \mathbf{I}) = {} & (-p - \lambda)[(-2 - \lambda)(-p - \lambda) - (p)(p)] \\ & - p[(p)(-p - \lambda) - (p)(0)] \\ & + 0[(p)(p) - (-2 - \lambda)(0)] \end{aligned}$$

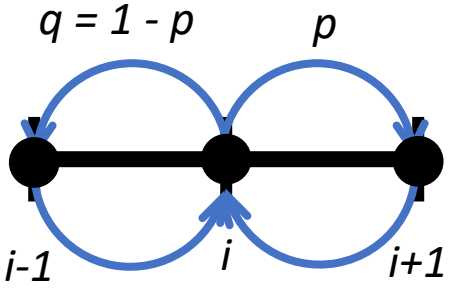
$$0 = 2p^3 - 2p^2 - 2\lambda^2 p + \lambda p^2 - 4p\lambda - \lambda^3 - 2\lambda^2$$

For p = 0.5

$$0 = 2p^3 - 2p^2 - 2\lambda^2 p + \lambda p^2 - 4p\lambda - \lambda^3 - 2\lambda^2$$

$$\lambda = -2.28, -0.5, -0.22$$

1D random walk



$$\begin{bmatrix}\dot{n}_{i-1}\\ \dot{n}_i\\ \dot{n}_{i+1}\end{bmatrix} = \begin{bmatrix}-p & p & 0\\ p & -2 & p\\ 0 & p & -p\end{bmatrix}\begin{bmatrix}n_{i-1}\\ n_i\\ n_{i+1}\end{bmatrix}$$

$$\dot{n}(t) = A(t)n(t)$$

$$\begin{bmatrix}-0.5-\lambda & 0.5 & 0\\ 0.5 & -2-\lambda & 0.5\\ 0 & 0.5 & -0.5-\lambda\end{bmatrix}\begin{bmatrix}n_{i-1}\\ n_i\\ n_{i+1}\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

$$\lambda = -2.28, -0.5, -0.22$$

Finding the **eigenvectors** (using scaled n-values)

$\boldsymbol{\lambda = -2.28}$

$$\begin{bmatrix}1.78 & 0.5 & 0\\ 0.5 & 0.28 & 0.5\\ 0 & 0.5 & 1.78\end{bmatrix}\begin{bmatrix}1\\ n_i\\ n_{i+1}\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

$$\mathbf{[1 \quad -3.56 \quad 1]^T}$$

$\boldsymbol{\lambda = -0.5}$

$$\begin{bmatrix}0 & 0.5 & 0\\ 0.5 & -1.5 & 0.5\\ 0 & 0.5 & 0\end{bmatrix}\begin{bmatrix}1\\ n_i\\ n_{i+1}\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

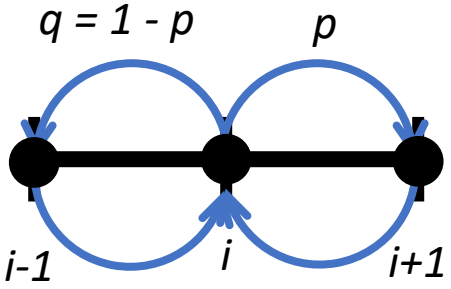
$$\mathbf{[1 \quad 0 \quad 1]^T}$$

$\boldsymbol{\lambda = -0.22}$

$$\begin{bmatrix}-0.28 & 0.5 & 0\\ 0.5 & -1.78 & 0.5\\ 0 & 0.5 & -0.28\end{bmatrix}\begin{bmatrix}1\\ n_i\\ n_{i+1}\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

$$\mathbf{[1 \quad 0.56 \quad 1]^T}$$

1D random walk



$\boldsymbol{\lambda = -2.28}$ $\quad [\mathbf{1} \quad \mathbf{-3.56} \quad \mathbf{1}]^{\mathsf{T}}$

$\boldsymbol{\lambda = -0.5}$ $\quad [\mathbf{1} \quad \mathbf{0} \quad \mathbf{1}]^{\mathsf{T}}$

$\boldsymbol{\lambda = -0.22}$ $\quad [\mathbf{1} \quad \mathbf{0.56} \quad \mathbf{1}]^{\mathsf{T}}$

Finding the **general solution** (using eigenvalues/vectors)

$$\mathbf{n(t)} = \sum_{k=1}^{N} c_k n_k e^{\lambda_k t}$$

$$\mathbf{n}(t) = c_1 e^{-2.28} \begin{bmatrix} 1 \\ -3.56 \\ 1 \end{bmatrix} + c_2 e^{-0.5} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + c_3\, e^{-0.22} \begin{bmatrix} 1 \\ 0.56 \\ 1 \end{bmatrix}$$

Use initial conditions to find solution (all *N* molecules start in position *i*)

$$\begin{bmatrix} 0 \\ N \\ 0 \end{bmatrix} = c_1 \begin{bmatrix} 1 \\ -3.56 \\ 1 \end{bmatrix} + c_2 \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + c_3 \begin{bmatrix} 1 \\ 0.56 \\ 1 \end{bmatrix}$$

1D random walk

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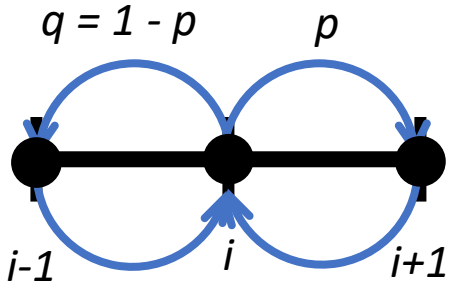
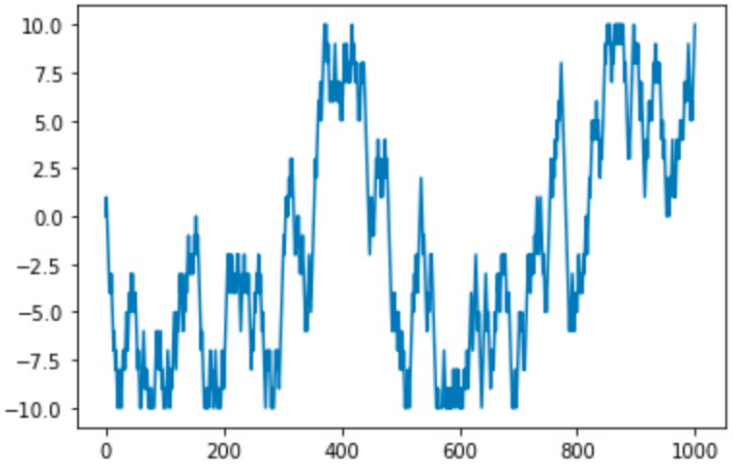
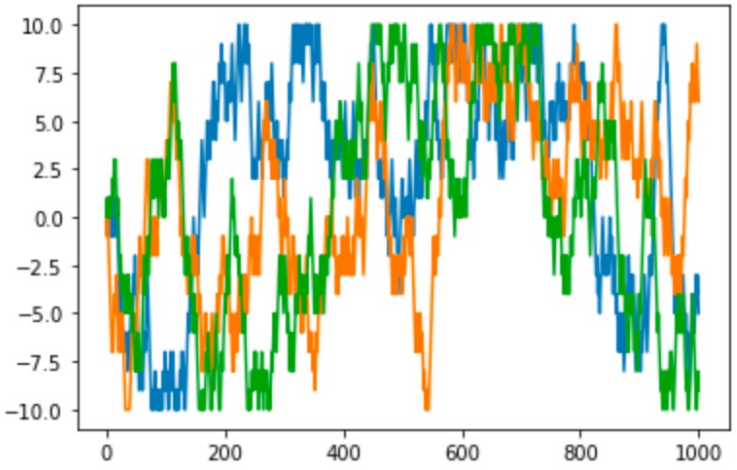


For a system with equal diffusivity in all directions, q = p = 0.5. 1000 time points in a range of x = [-10, 10]

1 molecule





3 molecules

Grid-free diffusion

Markovian model (1-D random walk)

- Random walk modeled as Markov process
- Flip a coin, move left or right
- Can be scaled to more molecules
- Requires a grid

Eigenmode analysis

- Grid-free analysis