Random Walk on Circle

Imagine a Markov process governing the random motion of a particle on a circular lattice:

The particle moves to the right or left with probability $\gamma$ and stays where it is with probability $1 - 2\gamma$. 
Random Walk on Circle (contd.)

The *random walk* can be defined as follows:

\[ p_{t+1}(i) = \sum_{j=0}^{N-1} p_{t+1|t}(i \mid j)p_t(j) \]

where

\[ p_{t+1|t}(i \mid j) = \begin{cases} 
(1 - 2\gamma) & \text{if } i = j \\
\gamma & \text{if } i = j \pm 1 \mod N \\
0 & \text{otherwise.}
\end{cases} \]

and \( i, j \in \{0, 1, \ldots, N - 1\} \).
Random Walk on Circle (contd.)

Because Markov processes are linear, the distribution at time $t + 1$ can be computed from the distribution at time $t$ by matrix vector product:

$$x^{(t+1)} = Px^{(t)}.$$  

Because the random walk is shift-invariant, the transition matrix $P$ is circulant:

$$P = \begin{bmatrix} (1 - 2\gamma) & \gamma & 0 & \cdots & 0 & \gamma \\ \gamma & (1 - 2\gamma) & \gamma & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \gamma & 0 & 0 & \cdots & \gamma & (1 - 2\gamma) \end{bmatrix}.$$
Diffusion in the Frequency Domain

Since $P$ is circulant, it is diagonalized by the DFT:

$$P = W \Lambda W^*$$

where the matrix $\Lambda$ contains the eigenvalues of $P$ on its diagonal:

$$\Lambda = \begin{bmatrix}
\lambda_0 & 0 & 0 & \ldots & 0 \\
0 & \lambda_1 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & \lambda_{N-1}
\end{bmatrix}.$$
Diffusion in the Frequency Domain (contd.)

Multiplying both sides of this expression by $W^*$ yields

$$ P = W\Lambda W^* $$
$$ W^*P = W^*W\Lambda W^* $$
$$ W^*P = \Lambda W^* $$
$$ W^*p_0 = \Lambda w^*_0 $$

where $p_0$ and $w^*_0$ are the first columns of $P$ and $W^*$. Since $w^*_0 = \frac{1}{\sqrt{N}}$ and $\Lambda$ is diagonal, it follows that

$$ w^* = \frac{1}{\sqrt{N}} \begin{bmatrix} (1 - 2\gamma) \\ \gamma \\ 0 \\ \vdots \\ 0 \\ \gamma \end{bmatrix} = \frac{1}{\sqrt{N}} \begin{bmatrix} \lambda_0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \lambda_{N-1} \end{bmatrix} + \frac{1}{\sqrt{N}} \begin{bmatrix} \lambda_1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \lambda_{N-1} \end{bmatrix} + \cdots + \frac{1}{\sqrt{N}} \begin{bmatrix} \lambda_N \end{bmatrix} $$
We see that the eigenvalues are $\sqrt{N}$ times the DFT of $P$'s first column:

$$\lambda_m = \gamma e^{-j2\pi m \frac{1}{N}} + (1 - 2\gamma) + \gamma e^{-j2\pi m \frac{(N-1)}{N}}.$$ 

Because $-(N-1) \mod N$ and $-1 = (N-1) \mod N$ are conjugate frequencies

$$e^{-j2\pi m \frac{(N-1)}{N}} + e^{-j2\pi m \frac{1}{N}} = 2\cos \left(2\pi m \frac{(N-1)}{N}\right).$$

Since $\gamma < 1/2$ and

$$0 < \cos \left(2\pi m \frac{(N-1)}{N}\right) < 1$$

for $0 < m < N - 1$, it follows that $\lambda_0 = 1$ and $0 < \lambda_m < 1$ for $m > 0$. 
The update equation for the Markov process looks like this:
\[ \mathbf{x}^{(t+1)} = \mathbf{W} \Lambda \mathbf{W}^* \mathbf{x}^{(t)}. \]

Because \( \Lambda \) is diagonal, higher powers of \( \mathbf{P} \) are easy to compute:
\[ \mathbf{P}^t = \mathbf{W} \Lambda^t \mathbf{W}^* \]
where
\[ \Lambda^t = \begin{bmatrix}
\lambda_{0}^{t} & 0 & 0 & \ldots & 0 \\
0 & \lambda_{1}^{t} & 0 & \ldots & 0 \\
0 & 0 & \lambda_{2}^{t} & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & \lambda_{N-1}^{t}
\end{bmatrix}. \]

Significantly, given an initial distribution, \( \mathbf{x}^{(0)} \), the distribution at any future time, \( \mathbf{x}^{(t)} \), can be computed by evaluating:
\[ \mathbf{x}^{(t)} = \mathbf{W} \Lambda^t \mathbf{W}^* \mathbf{x}^{(0)}. \]
Limiting Distribution of Diffusion Process

Taking the limit as $t$ goes to infinity yields
\[
\lim_{t \to \infty} x(t) = \lim_{t \to \infty} W \Lambda^t W^* x^{(0)}
\]
\[
= \lim_{t \to \infty} \left( \sum_{m=0}^{N-1} \lambda_m^t w_m w_m^H \right) x^{(0)}
\]

where $H$ is conjugate transpose. Since $\lambda_0 = 1$ and $\lim_{t \to \infty} \lambda_m = 0$ for $m \neq 0$ it follows that
\[
\lim_{t \to \infty} x(t) = w_0 w_0^H x^{(0)}
\]
\[
= \frac{1}{N} \mathbf{1}
\]

because $w_0 = \frac{1}{\sqrt{N}} \mathbf{1}$, and $\sum_{n=0}^{n-1} x_n = 1$. We see that probability mass is uniformly distributed among the sites in the ring.
Diffusion Equation

The following expression for $P_{x}^{t+1}$ in terms of $P_{x}^{t}, P_{x+1}^{t}$, and $P_{x-1}^{t}$ is termed the master equation for the diffusion process:

$$P_{x}^{t+1} = P_{x}^{t} - 2\gamma P_{x}^{t} + \gamma P_{x-1}^{t} + \gamma P_{x+1}^{t}$$

where $2\gamma P_{x}^{t}$ is the probability mass which leaves $P_{x}^{t}$ in one step and $\gamma P_{x-1}^{t} + \gamma P_{x+1}^{t}$ is the probability mass which enters $P_{x}^{t}$ in one step.
The above expression for $\Delta t = \Delta x = 1$ can be generalized for arbitrary $\Delta t$ and $\Delta x$ by defining $\gamma = D\frac{\Delta t}{(\Delta x)^2}$:

$$P_x^{t+\Delta t} = P_x^t - \underbrace{2DP_x^t \frac{\Delta t}{(\Delta x)^2}}_{\text{out}} + \underbrace{DP_{x-\Delta x}^t \frac{\Delta t}{(\Delta x)^2} + DP_{x+\Delta x}^t \frac{\Delta t}{(\Delta x)^2}}_{\text{in}}$$

where $D$ is termed the diffusion constant. Solving for $(P_x^{t+\Delta t} - P_x^t) / \Delta t$ yields:

$$\frac{(P_x^{t+\Delta t} - P_x^t)}{\Delta t} = \left( DP_{x+\Delta x}^t - 2DP_x^t + DP_{x-\Delta x}^t \right) / (\Delta x)^2$$

$$= \left( DP_{x+\Delta x}^t - DP_x^t + DP_{x-\Delta x}^t - DP_x^t \right) / (\Delta x)^2$$
Diffusion Equation (contd.)

\[
\frac{(P_{x}^{t+\Delta t} - P_{x}^{t})}{\Delta t} = D \left( \frac{P_{x+\Delta x}^{t} - P_{x}^{t} + P_{x-\Delta x}^{t} - P_{x}^{t}}{(\Delta x)^{2}} \right)
\]

which can be rewritten as follows:

\[
\frac{P_{x}^{t+\Delta t} - P_{x}^{t}}{\Delta t} = D \left[ \frac{P_{x+\Delta x}^{t} - P_{x}^{t}}{\Delta x} - \frac{P_{x}^{t} - P_{x-\Delta x}^{t}}{\Delta x} \right].
\]
Diffusion Equation (contd.)

Taking the limit as $\Delta x = \Delta t \to 0$:

$$
\lim_{\Delta t \to 0} \frac{(P_{x}^{t+\Delta t} - P_{x}^{t})}{\Delta t} = \lim_{\Delta x \to 0} D \left[ \frac{(P_{x+\Delta x}^{t} - P_{x}^{t})}{\Delta x} - \frac{(P_{x}^{t} - P_{x-\Delta x}^{t})}{\Delta x} \right]
$$

yields a *partial differential equation (PDE)*:

$$
\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}
$$

which is known as the *diffusion equation*.
Green’s Function

\[
\frac{\partial P(x, t)}{\partial t} = \frac{\partial^2 P(x, t)}{\partial x^2}
\]

\[
\frac{\partial}{\partial t} \left( \frac{1}{\sqrt{4\pi t}} e^{-x^2/4t} \right)
= \frac{\partial^2}{\partial x^2} \left( \frac{1}{\sqrt{4\pi t}} e^{-x^2/4t} \right)
\]

\[
\frac{(x^2 - 2t) e^{-x^2/4t}}{8 \sqrt{\pi} t^{5/2}}
= \frac{(x^2 - 2t) e^{-x^2/4t}}{8 \sqrt{\pi} t^{5/2}}
\]
Finite Difference Approximation of $\frac{\partial P}{\partial x}$

The value of the function, $P$, at the point, $(x + \Delta x, t)$, can be expressed as a Taylor series expansion about the point, $(x, t)$, as follows:

$$P_{t,x+\Delta x} = P_{t,x} + \Delta x \left. \frac{\partial P}{\partial x} \right|_{x,t} + \frac{(\Delta x)^2}{2!} \left. \frac{\partial^2 P}{\partial x^2} \right|_{x,t} + O[(\Delta x)^3].$$

By rearranging the above, we derive the \textit{forward difference} approximation for $\frac{\partial P}{\partial x}|_{x,t}$:

$$\frac{P_{t,x+\Delta x} - P_{t,x}}{\Delta x} = \left. \frac{\partial P}{\partial x} \right|_{x,t} + O[\Delta x].$$
Backward Difference Approximation of $\frac{\partial P}{\partial x}$

The value of the function, $P$, at the point, $(x - \Delta x, t)$, can be expressed as a Taylor series expansion about the point, $(x, t)$, as follows:

$$P_{x-\Delta x}^t = P_x^t - \Delta x \frac{\partial P}{\partial x}\bigg|_{x,t} + \frac{(-\Delta x)^2}{2!} \frac{\partial^2 P}{\partial x^2}\bigg|_{x,t} + O[(\Delta x)^3].$$

By rearranging the above, we derive the \textit{backward difference} approximation for $\frac{\partial P}{\partial x}\big|_{x,t}$:

$$\frac{P_x^t - P_{x-\Delta x}^t}{\Delta x} = \frac{\partial P}{\partial x}\bigg|_{x,t} + O[\Delta x].$$
Centered Difference Approximation of $\frac{\partial P}{\partial x}$

\[ P_{x+\Delta x}^t = P_x^t + \Delta x \left. \frac{\partial P}{\partial x} \right|_{x,t} + \frac{(\Delta x)^2}{2!} \left. \frac{\partial^2 P}{\partial x^2} \right|_{x,t} + \frac{(\Delta x)^3}{3!} \left. \frac{\partial^3 P}{\partial x^3} \right|_{x,t} + O[(\Delta x)^4] \]

\[ P_{x-\Delta x}^t = P_x^t - \Delta x \left. \frac{\partial P}{\partial x} \right|_{x,t} + \frac{(-\Delta x)^2}{2!} \left. \frac{\partial^2 P}{\partial x^2} \right|_{x,t} + \frac{(-\Delta x)^3}{3!} \left. \frac{\partial^3 P}{\partial x^3} \right|_{x,t} + O[(\Delta x)^4] \]

Subtracting $P_{x-\Delta x}^t$ from $P_{x+\Delta x}^t$ yields:

\[ P_{x+\Delta x}^t - P_{x-\Delta x}^t = 2\Delta x \left. \frac{\partial P}{\partial x} \right|_{x,t} + 2 \frac{(-\Delta x)^3}{3!} \left. \frac{\partial^3 P}{\partial x^3} \right|_{x,t} + O[(\Delta x)^4]. \]
Centered Difference Approx. of $\frac{\partial P}{\partial x}$ (contd.)

This can be rearranged to yield the centered difference approximation for $\frac{\partial P}{\partial x}$:

$$\frac{P_{x+\Delta x}^t - P_{x-\Delta x}^t}{2\Delta x} = \frac{\partial P}{\partial x} \bigg|_{x,t} + O[(\Delta x)^2].$$

Notice that the centered difference approximation is second order accurate.
Finite Difference Approximation of $\frac{\partial^2 P}{\partial x^2}$

The value of the function, $\frac{\partial P}{\partial x}$, at the point, $(x + \Delta x, t)$, can be expressed as a Taylor series expansion about the point, $(x, t)$, as follows:

$$\left. \frac{\partial P}{\partial x} \right|_{x+\Delta x, t} = \left. \frac{\partial P}{\partial x} \right|_{x, t} + \Delta x \left. \frac{\partial^2 P}{\partial x^2} \right|_{x, t} + \frac{(\Delta x)^2}{2!} \left. \frac{\partial^3 P}{\partial x^3} \right|_{x, t} + O[(\Delta x)^3].$$

Given the above we can derive the forward difference approximation for $\left. \frac{\partial^2 P}{\partial x^2} \right|_{x, t}$:

$$\frac{\frac{\partial P}{\partial x}|_{x+\Delta x, t} - \frac{\partial P}{\partial x}|_{x, t}}{\Delta x} = \left. \frac{\partial^2 P}{\partial x^2} \right|_{x, t} + O[\Delta x].$$
Finite Difference Approx. of $\frac{\partial^2 P}{\partial x^2}$ (contd.)

For reasons of symmetry, we approximate $\frac{\partial P}{\partial x}|_{x+\Delta x,t}$ and $\frac{\partial P}{\partial x}|_{x,t}$ using backward differences:

$$\left[\frac{P_{x+\Delta x}^t - P_x^t}{\Delta x} - \frac{P_x^t - P_{x-\Delta x}^t}{\Delta x}\right] = \frac{\Delta x}{\Delta x}$$

$$\left.\frac{\partial^2 P}{\partial x^2}\right|_{x,t} + O[\Delta x].$$

Combining terms yields the following expression for $\left.\frac{\partial^2 P}{\partial x^2}\right|_{x,t}$:

$$\frac{P_{x+\Delta x}^t - 2P_x^t + P_{x-\Delta x}^t}{(\Delta x)^2} = \left.\frac{\partial^2 P}{\partial x^2}\right|_{x,t} + O[\Delta x].$$
Diffusion Equation (reprise)

Applying the finite difference approximations we’ve derived to the diffusion equation:

\[ \frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2} \]

yields

\[ \frac{P_{x}^{t+\Delta t} - P_{x}^{t}}{\Delta t} = D \left( \frac{P_{x+\Delta x}^{t} - 2P_{x}^{t} + P_{x-\Delta x}^{t}}{(\Delta x)^2} \right) \]

which can be re-arranged to yield:

\[ \frac{P_{x}^{t+\Delta t} - P_{x}^{t}}{\Delta t} = D \frac{\left[ \frac{P_{x+\Delta x}^{t} - P_{x}^{t}}{\Delta x} - \frac{P_{x}^{t} - P_{x-\Delta x}^{t}}{\Delta x} \right]}{\Delta x} \]

which (we recall) is equivalent to the master equation:

\[ P_{x}^{t+\Delta t} = P_{x}^{t} - 2DP_{x}^{t} \frac{\Delta t}{(\Delta x)^2} + DP_{x-\Delta x}^{t} \frac{\Delta t}{(\Delta x)^2} + DP_{x+\Delta x}^{t} \frac{\Delta t}{(\Delta x)^2}. \]
Wave Equation

The partial differential equation governing wave motion is:

\[
\frac{\partial^2 P}{\partial t^2} = c^2 \frac{\partial^2 P}{\partial x^2}.
\]

Applying the finite difference approximations for \( \frac{\partial^2 P}{\partial t^2} \big|_{x,t} \) and \( \frac{\partial^2 P}{\partial x^2} \big|_{x,t} \) yields:

\[
P_{x}^{t+\Delta t} - 2P_{x}^{t} + P_{x}^{t-\Delta t}
\]

\[
(\Delta t)^2
\]

\[
\approx c^2 \left( \frac{P_{x+\Delta x}^{t} - 2P_{x}^{t} + P_{x-\Delta x}^{t}}{(\Delta x)^2} \right).
\]

Solving for \( P_{x}^{t+\Delta t} \) gives the following update formula:

\[
P_{x}^{t+\Delta t} = -P_{x}^{t-\Delta t} +
\]

\[
2 \left[ 1 - c^2 \left( \frac{\Delta t}{\Delta x} \right)^2 \right] P_{x}^{t} + c^2 \left( \frac{\Delta t}{\Delta x} \right)^2 \left( P_{x+\Delta x}^{t} + P_{x-\Delta x}^{t} \right).
\]
First Order in Time

Unfortunately, this formula is second-order in time. To derive a formula which is first-order in time, we recall that

$$\frac{\partial^2 P}{\partial t^2} \bigg|_{x,t} = \frac{\partial P}{\partial t} \bigg|_{x,t+\Delta t} - \frac{\partial P}{\partial t} \bigg|_{x,t} + \mathcal{O}[\Delta t].$$

Replacing $\frac{\partial P}{\partial t} \bigg|_{x,t+\Delta t}$ with $\frac{P_{x+\Delta t}^t - P_x^t}{\Delta t}$ and using the resulting expression for $\frac{\partial^2 P}{\partial t^2} \bigg|_{x,t}$ and a centered difference approximation for $\frac{\partial^2 P}{\partial x^2} \bigg|_{x,t}$ in the wave equation yields:

$$\frac{P_{x+\Delta t}^t - P_x^t}{\Delta t} - \frac{\partial P}{\partial t} \bigg|_{x,t} \approx c^2 \left( \frac{P_{x+\Delta x}^t - 2P_x^t + P_{x-\Delta x}^t}{(\Delta x)^2} \right).$$

Multiplying both sides by $\Delta t$:

$$\frac{P_{x+\Delta t}^t - P_x^t}{\Delta t} - \dot{P}_x^t \approx c^2 \left( \frac{\Delta t}{(\Delta x)^2} \left( P_{x+\Delta x}^t - 2P_x^t + P_{x-\Delta x}^t \right) \right).$$
First Order in Time (contd.)

Multiplying both sides by $\Delta t$ again, and then adding $P^t_x$ and $\Delta t \dot{P}^t_x$ to both sides yields:

$$P^{t+\Delta t}_x \approx P^t_x + \Delta t \dot{P}^t_x$$

$$+ c^2 \left( \frac{\Delta t}{\Delta x} \right)^2 \left( P^t_{x+\Delta x} - 2P^t_x + P^t_{x-\Delta x} \right)$$

which can be rearranged to give an update equation for $P$ which is first-order in time:

$$P^{t+\Delta t}_x = \left[ 1 - 2c^2 \left( \frac{\Delta t}{\Delta x} \right)^2 \right] P^t_x + \Delta t \dot{P}^t_x$$

$$+ c^2 \left( \frac{\Delta t}{\Delta x} \right)^2 \left( P^t_{x+\Delta x} + P^t_{x-\Delta x} \right).$$
First Order in Time (contd.)

To derive an update equation for \( \dot{P} \) which is also first-order in time, we once again begin with

\[
\frac{\partial^2 P}{\partial t^2} \bigg|_{x,t} = \frac{\partial P}{\partial t} \bigg|_{x,t+\Delta t} - \frac{\partial P}{\partial t} \bigg|_{x,t} / \Delta t + O[\Delta t].
\]

Using the above and a centered difference approximation for \( \frac{\partial^2 P}{\partial x^2} \bigg|_{x,t} \) in the wave equation results in:

\[
\frac{\partial P}{\partial t} \bigg|_{x,t+\Delta t} - \frac{\partial P}{\partial t} \bigg|_{x,t} / \Delta t \approx c^2 \left( \frac{P_{x+\Delta x}^t - 2P_x^t + P_{x-\Delta x}^t}{(\Delta x)^2} \right).
\]

Writing \( \dot{P}_x^t \) for \( \frac{\partial P}{\partial t} \bigg|_{x,t} \) yields the following update equation for \( \dot{P} \):

\[
\dot{P}_{x}^{t+\Delta t} = \dot{P}_x^t + c^2 \frac{\Delta t}{(\Delta x)^2} \left( P_{x+\Delta x}^t - 2P_x^t + P_{x-\Delta x}^t \right).
\]

We observe that the update equations for both \( P \) and \( \dot{P} \) are first-order in time.