One-dimensional Random Walk

Consider the following Markov process:

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

where \( i, j \in \{0, 1, \ldots, N - 1\} \) and

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

All of this can be expressed more concisely in matrix notation:

\[ \mathbf{x}^{(t+1)} = \mathbf{P}\mathbf{x}^{(t)} \]

where \( \mathbf{P} \) is a stochastic matrix:

\[
\mathbf{P} = \begin{bmatrix}
(1 - 2\gamma) & \gamma & 0 & \ldots & 0 & \gamma \\
\gamma & (1 - 2\gamma) & \gamma & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\gamma & 0 & 0 & \ldots & \gamma & (1 - 2\gamma)
\end{bmatrix}.
\]

Because the random walk is shift-invariant, \( \mathbf{P} \) is circulant.
Diffusion in the Frequency Domain

It follows that $\mathbf{P}$ is diagonalized by the DFT:

$$\mathbf{P} = \mathbf{W} \Lambda \mathbf{W}^*.$$  

The matrix $\Lambda$ contains the eigenvalues of $\mathbf{P}$ on its diagonal:

$$\Lambda = \begin{bmatrix} 
\lambda_0 & 0 & 0 & \ldots & 0 \\
0 & \lambda_1 & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & \lambda_{N-1} 
\end{bmatrix}.$$  

where $\lambda_0, \ldots, \lambda_{N-1}$ are the (unnormalized) DFT of the first column of $\mathbf{P} = [p_{ij}]$:

$$\lambda_m = \sum_{n=0}^{N-1} p_{n0} e^{-j2\pi m \frac{n}{N}}$$

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

which is real.
Diffusion in the Frequency Domain (contd.)

The update equation for the Markov chain looks like this:

\[ x^{(t+1)} = W \Lambda W^* x^{(t)}. \]

Higher powers of \( P \) are easy to compute:

\[ P^t = W \Lambda^t W^* \]

where

\[
\Lambda^t = \begin{bmatrix}
\lambda_0^t & 0 & 0 & \ldots & 0 \\
0 & \lambda_1^t & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & \lambda_{N-1}^t
\end{bmatrix}.
\]

Finally, given an initial distribution, \( x^{(0)} \), the distribution at time, \( t \), is:

\[ x^{(t)} = W \Lambda^t W^* x^{(0)}. \]
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.
Diffusion Equation (contd.)

The above expression for $\Delta t = \Delta x = 1$ can be generalized for arbitrary $\Delta t$ and $\Delta x$ by defining $\gamma = D \frac{\Delta t}{(\Delta x)^2}$:

$$P_{x}^{t+\Delta t} = P_{x}^{t} -$$

$$2DP_{x}^{t} \frac{\Delta t}{(\Delta x)^2} + DP_{x-\Delta x}^{t} \frac{\Delta t}{(\Delta x)^2} + DP_{x+\Delta x}^{t} \frac{\Delta t}{(\Delta x)^2}$$

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

$$\frac{(P_{x}^{t+\Delta t} - P_{x}^{t})}{\Delta t}$$

$$= \frac{(DP_{x+\Delta x}^{t} - 2DP_{x}^{t} + DP_{x-\Delta x}^{t})}{(\Delta x)^2}$$

$$= \frac{(DP_{x+\Delta x}^{t} - DP_{x}^{t} + DP_{x-\Delta x}^{t} - DP_{x}^{t})}{(\Delta x)^2}$$
Diffusion Equation (contd.)

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

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 $\Delta x = \Delta t \to 0$:

$$\lim_{\Delta t \to 0} \frac{\left( P_x^{t+\Delta t} - P_x^t \right)}{\Delta t} =$$

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

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.
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:

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

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

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

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

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

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

\[ P^t_{x+\Delta x} = P^t_x + \Delta x \frac{\partial P}{\partial x} \bigg|_{x,t} + \frac{(\Delta x)^2}{2!} \frac{\partial^2 P}{\partial x^2} \bigg|_{x,t} + \frac{(\Delta x)^3}{3!} \frac{\partial^3 P}{\partial x^3} \bigg|_{x,t} + O[(\Delta x)^4] \]

\[ P^t_{x-\Delta x} = P^t_x - \Delta x \frac{\partial P}{\partial x} \bigg|_{x,t} + \frac{(-\Delta x)^2}{2!} \frac{\partial^2 P}{\partial x^2} \bigg|_{x,t} + \frac{(-\Delta x)^3}{3!} \frac{\partial^3 P}{\partial x^3} \bigg|_{x,t} + O[(\Delta x)^4] \]

Subtracting $P^t_{x-\Delta x}$ from $P^t_{x+\Delta x}$ yields:

\[ P^t_{x+\Delta x} - P^t_{x-\Delta x} = 2\Delta x \frac{\partial P}{\partial x} \bigg|_{x,t} + 2 \frac{(-\Delta x)^3}{3!} \frac{\partial^3 P}{\partial x^3} \bigg|_{x,t} + O[(\Delta x)^4]. \]
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, $\partial P / \partial x$, at the point, $(x + \Delta x, t)$, can be expressed as a Taylor series expansion about the point, $(x, t)$, as follows:

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

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

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

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

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

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

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

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 \(\frac{\partial^2 P}{\partial t^2}|_{x,t}\) and \(\frac{\partial^2 P}{\partial x^2}|_{x,t}\) yields:

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

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

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

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

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

Multiplying both sides by \(\Delta t\):

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

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

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

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

Writing $\dot{P}^t_x$ for $\frac{\partial P}{\partial t}|_{x,t}$ yields the following update equation for $\dot{P}$:

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

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