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 $i, j \in \{0, 1, ..., N-1\}$ and

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

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 Λ contains the eigenvalues of $\mathbf{P}$ on its diagonal:

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

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

$$\begin{aligned} \lambda_m &= \sum_{n=0}^{N-1} p_{n\,0}\, e^{-j2\pi m \frac{n}{N}} \\ &= (1-2\gamma) + \gamma e^{-j2\pi m \frac{1}{N}} + \gamma e^{-j2\pi m \frac{(N-1)}{N}}. \end{aligned}$$

which is real.

Diffusion in the Frequency Domain (contd.)

The update equation for the Markov chain looks like this:

$$\mathbf{x}^{(t+1)} = \mathbf{W}\Lambda\mathbf{W}^*\mathbf{x}^{(t)}.$$

Higher powers of $\mathbf{P}$ are easy to compute:

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

where

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

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

$$\mathbf{x}^{(t)} = \mathbf{W}\Lambda^t\mathbf{W}^*\mathbf{x}^{(0)}.$$

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 Δt and Δx 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 $\left(P_x^{t+\Delta t} - P_x^t\right)/\Delta t$ yields:

$$\left(P_x^{t+\Delta t} - P_x^t\right)/\Delta t$$

$$\begin{aligned} &= \left(DP_{x+\Delta x}^t - 2DP_x^t + DP_{x-\Delta x}^t\right)/(\Delta x)^2 \\ &= \left(DP_{x+\Delta x}^t - DP_x^t + DP_{x-\Delta x}^t - DP_x^t\right)/(\Delta x)^2 \end{aligned}$$

Diffusion Equation (contd.)

$$\left(P_x^{t+\Delta t} - P_x^t\right)/\Delta t$$

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

which can be rewritten as follows:

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

Diffusion Equation (contd.)

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

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

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

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:

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

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

$$\frac{P^t_{x+\Delta x} - P^t_x}{\Delta x} = \left.\frac{\partial P}{\partial x}\right|_{x,t} + \mathrm{O}[\Delta x].$$

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:

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

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

$$\frac{P^t_x - P^t_{x-\Delta x}}{\Delta x} = \left.\frac{\partial P}{\partial x}\right|_{x,t} + \mathrm{O}[\Delta x].$$

Centered Difference Approximation of $\frac{\partial P}{\partial x}$

$$P^{t}_{x+\Delta x} = P^{t}_{x} +$$

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

$$P^{t}_{x-\Delta x} = P^{t}_{x} -$$

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

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

$$P^{t}_{x+\Delta x} - P^{t}_{x-\Delta x} = 2\Delta x \left.\frac{\partial P}{\partial x}\right|_{x,t} +$$

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

Centered Difference Approx. of $\frac{\partial P}{\partial x}$ (contd.)

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

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

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:

$$\left.\frac{\partial P}{\partial x}\right|_{x+\Delta x,t} = \left.\frac{\partial P}{\partial x}\right|_{x,t} +$$

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

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

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

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:

$$\frac{\left[\frac{P^t_{x+\Delta x}-P^t_x}{\Delta x} - \frac{P^t_x-P^t_{x-\Delta x}}{\Delta x}\right]}{\Delta x} =$$

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

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

$$\frac{P^t_{x+\Delta x} - 2P^t_x + P^t_{x-\Delta x}}{(\Delta x)^2} =$$

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

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

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

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

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

Replacing $\frac{\partial P}{\partial t}|_{x,t+\Delta t}$ with $\frac{P_x^{t+\Delta t} - P_x^t}{\Delta t}$ 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:

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

Multiplying both sides by Δt:

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

First Order in Time (contd.)

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

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

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

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

First Order in Time (contd.)

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

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

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

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

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

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

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