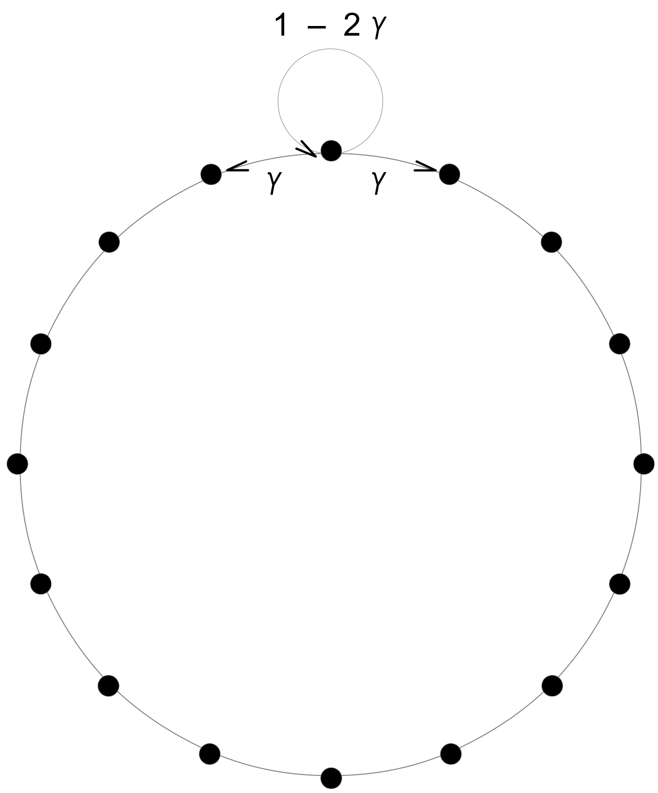
Random Walk on Circle

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 γ 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

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

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:

$$\mathbf{x}^{(t+1)} = \mathbf{P}\mathbf{x}^{(t)}.$$

Because the random walk is shift-invariant, the transition matrix $\mathbf{P}$ is circulant:

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

Diffusion in the Frequency Domain

Since $\mathbf{P}$ is circulant, it is diagonalized by the DFT:

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

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

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

Diffusion in the Frequency Domain (contd.)

Multiplying both sides of this expression by $\mathbf{W}^*$ yields

$$\begin{aligned}
\mathbf{P} &= \mathbf{W}\Lambda\mathbf{W}^* \\
\mathbf{W}^*\mathbf{P} &= \mathbf{W}^*\mathbf{W}\Lambda\mathbf{W}^* \\
\mathbf{W}^*\mathbf{P} &= \Lambda\mathbf{W}^* \\
\mathbf{W}^*\mathbf{p}_0 &= \Lambda\mathbf{w}_0^*
\end{aligned}$$

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

$$\begin{aligned}
\mathbf{W}^* \begin{bmatrix} (1-2\gamma) \\ \gamma \\ 0 \\ \vdots \\ 0 \\ \gamma \end{bmatrix} &= \frac{1}{\sqrt{N}} \begin{bmatrix} \lambda_0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \frac{1}{\sqrt{N}} \begin{bmatrix} 0 \\ \lambda_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \cdots + \frac{1}{\sqrt{N}} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \lambda_{N-1} \end{bmatrix} \\
&= \frac{1}{\sqrt{N}} \begin{bmatrix} \lambda_0 \\ \lambda_1 \\ \vdots \\ \lambda_{N-1} \end{bmatrix}.
\end{aligned}$$

Diffusion in the Frequency Domain (contd.)

We see that the eigenvalues are $\sqrt{N}$ times the DFT of $\mathbf{P}$'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 $m > 0$.

Diffusion in the Frequency Domain (contd.)

The update equation for the Markov process looks like this:

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

Because Λ is diagonal, higher powers of $\mathbf{P}$ are easy to compute:

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

where

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

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

$$\begin{aligned}\lim_{t\to\infty}\mathbf{x}^{(t)} &= \lim_{t\to\infty}\mathbf{W}\Lambda^t\mathbf{W}^*\mathbf{x}^{(0)} \\ &= \lim_{t\to\infty}\left(\sum_{m=0}^{N-1}\lambda_m^t\mathbf{w}_m\mathbf{w}_m^{\mathrm{H}}\right)\mathbf{x}^{(0)}\end{aligned}$$

where H is conjugate transpose. Since $\lambda_0 = 1$ and $\lim_{t\to\infty}\lambda_m = 0$ for $m \neq 0$ it follows that

$$\begin{aligned}\lim_{t\to\infty}\mathbf{x}^{(t)} &= \mathbf{w}_0\mathbf{w}_0^{\mathrm{H}}\mathbf{x}^{(0)} \\ &= \frac{1}{N}\,\mathbf{1}\end{aligned}$$

because $\mathbf{w}_0 = \frac{1}{\sqrt{N}}\mathbf{1}$, 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.

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.)

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

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

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.*

Green's Function

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

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

$$\frac{\left(x^2 - 2t\right) e^{-x^2/4t}}{8\sqrt{\pi}\, t^{5/2}} = \frac{\left(x^2 - 2t\right) e^{-x^2/4t}}{8\sqrt{\pi}\, t^{5/2}}$$

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:

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

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

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

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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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.