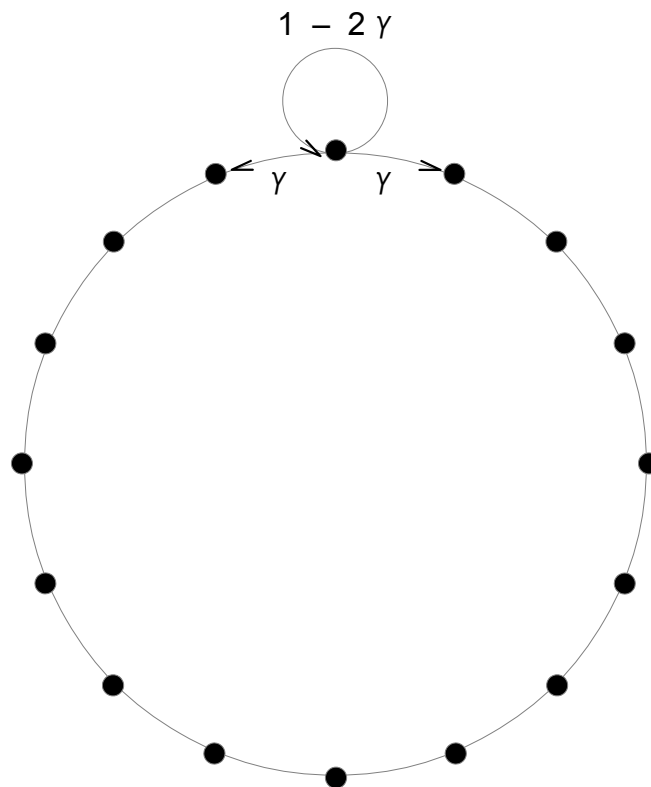


## Random Walk on Circle

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:

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

where

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

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

## 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:

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

## Diffusion in the Frequency Domain

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

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

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

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

## Diffusion in the Frequency Domain (contd.)

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

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

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

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

$$\mathbf{W}^*\mathbf{p}_0 = \Lambda\mathbf{w}_0^*$$

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  $\Lambda$  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  $-(N-1) \bmod N$  and  $-1 = (N-1) \bmod N$  are conjugate frequencies

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

It follows that the eigenvalues of  $\mathbf{P}$  are real. 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  $\Lambda$  is diagonal, higher powers of  $\mathbf{P}$  are easy to compute:

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

where

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

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

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

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

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

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  $\Delta t$  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:

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

## Diffusion Equation (contd.)

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

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

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

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:

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

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

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

## 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:

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

## Finite Difference Approx. of $\frac{\partial^2 P}{\partial x^2}$ (contd.)

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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:

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

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

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

## 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:

$$P_x^{t+\Delta t} = P_x^t - 2D P_x^t \frac{\Delta t}{(\Delta x)^2} + D P_{x-\Delta x}^t \frac{\Delta t}{(\Delta x)^2} + D P_{x+\Delta x}^t \frac{\Delta t}{(\Delta x)^2}.$$

## 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:

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

## 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

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

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

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

## First Order in Time (contd.)

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

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

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

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

## 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

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

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

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

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

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

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