From random walk to diffusion equation

Diffusion equation

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- The *Laplacian*, Δu, is defined by $\Delta u = u_{xx} + u_{yy}$.
- One can also consider the diffusion equation *with drift and reaction*:

$$u_t = k\Delta u + \boldsymbol{b} \cdot \nabla u - \gamma u$$

Symmetric multidimensional random walk - set up

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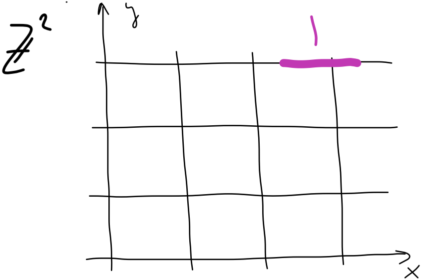
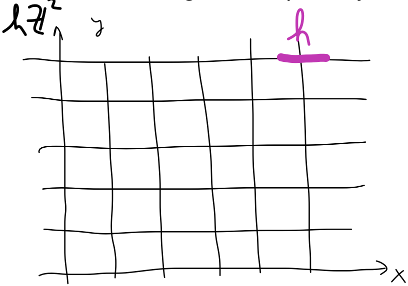
- Lattice $h\mathbb{Z}^2$is the set of points whose coordinates are integers multiplied by h.





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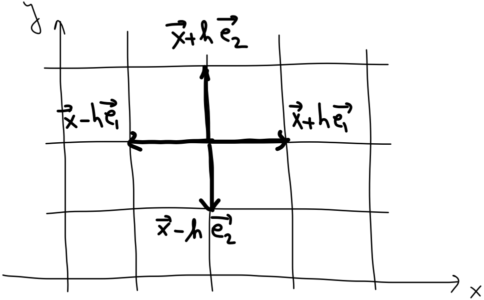
If we denote by $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ the basis of $\mathbb{R}^2$, every point $\boldsymbol{x} \in h\mathbb{Z}^2$, has a discrete neighborhood of 4 points at distance h, given by:

$$\boldsymbol{x} + h\boldsymbol{e}_1, \quad \boldsymbol{x} - h\boldsymbol{e}_1, \quad \boldsymbol{x} + h\boldsymbol{e}_2, \quad \boldsymbol{x} - h\boldsymbol{e}_2.$$

Symmetric multidimensional random walk -rules



The particle moves according to the following rules:

1. It starts from $\boldsymbol{x} = \mathbf{0}$.
2. If at time t, the particle is located at $\boldsymbol{x}$, then at time $t + \tau$ it is at one of the four neighboring points $\boldsymbol{x} \pm h\boldsymbol{e}_1$, $\boldsymbol{x} \pm h\boldsymbol{e}_2$, with probability $\frac{1}{4}$.
3. Each step is independent of the previous one.

Symmetric multidimensional random walk - probability

We now calculate the probability $p(\boldsymbol{x}, t)$ of finding the particle at position $\boldsymbol{x}$ at time t. This probability has the following initial conditions: $p(\mathbf{0}, 0) = 1$ and $p(\boldsymbol{x}, 0) = 0$ if $\boldsymbol{x} \neq 0$.

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$$p(\boldsymbol{x}, t+\tau) = \frac{1}{4} \sum_{j=1}^{2} \Big(p(\boldsymbol{x} + h\boldsymbol{e_j}, t) + p(\boldsymbol{x} - h\boldsymbol{e_j}, t) \Big).$$

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For fixed $\boldsymbol{x}$ and t, we want to find the limit as $h \to 0$ and $\tau \to 0$. Assuming p is defined and smooth, by Taylor's formula we have:

$$\begin{aligned}
p(\boldsymbol{x}, t+\tau) &= p(\boldsymbol{x}, t) + p_t(\boldsymbol{x}, t)\tau + o(\tau) \\
p(\boldsymbol{x}+h\boldsymbol{e_j}, t) &= p(\boldsymbol{x}, t) + p_{x_j}(\boldsymbol{x}, t)h + \frac{1}{2}p_{x_jx_j}(\boldsymbol{x}, t)h^2 + o(h^2) \\
p(\boldsymbol{x}-h\boldsymbol{e_j}, t) &= p(\boldsymbol{x}, t) - p_{x_j}(\boldsymbol{x}, t)h + \frac{1}{2}p_{x_jx_j}(\boldsymbol{x}, t)h^2 + o(h^2)
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Combining the last four formulas, we have:

$$p(\boldsymbol{x}, t) + p_t(\boldsymbol{x}, t)\tau + o(\tau) = \frac{1}{4}\sum_{j=1}^{2}\Big(2p(\boldsymbol{x}, t) + p_{x_jx_j}(\boldsymbol{x}, t)h^2 + o(h^2)\Big)$$

Symmetric multidimensional random walk - probability

Therefore, after canceling $p(\boldsymbol{x}, t)$ and dividing by τ:

$$p_t + o(1) = \frac{1}{4}\frac{h^2}{\tau}\Delta p + o(\frac{h^2}{\tau}).$$

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To obtain nontrivial limit, $\frac{h^2}{\tau}$ must have a finite and positive limit. The simplest choice is to set the ratio to be equal to a constant:

$$\frac{h^2}{\tau} = 4k, \qquad k > 0.$$

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with the initial condition

$$\lim_{t \to 0+} p(\boldsymbol{x}, t) = \delta.$$

In this limit, the random walk has become a continuous walk. If $k = 1$, it is called (2-dimensional) Brownian motion.

Walks with different space steps

One variant of a symmetric random walk is to choose a different space step h_j for every direction $\boldsymbol{e_j}$, i.e. space step h_1 for direction $\boldsymbol{e_1}$ and space step h_2 for direction $\boldsymbol{e_2}$.

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For fixed $\boldsymbol{x}$ and t, we want to find the limit as $h_j \to 0$ and $\tau \to 0$. By Taylor's formula we have:

$$p(\boldsymbol{x}, t+\tau) = p(\boldsymbol{x}, t) + p_t(\boldsymbol{x}, t)\tau + o(\tau)$$

$$p(\boldsymbol{x} + h_j\boldsymbol{e_j}, t) = p(\boldsymbol{x}, t) + p_{x_j}(\boldsymbol{x}, t)h_j + \frac{1}{2}p_{x_jx_j}(\boldsymbol{x}, t){h_j}^2 + o({h_j}^2)$$

$$p(\boldsymbol{x} - h_j\boldsymbol{e_j}, t) = p(\boldsymbol{x}, t) - p_{x_j}(\boldsymbol{x}, t)h_j + \frac{1}{2}p_{x_jx_j}(\boldsymbol{x}, t){h_j}^2 + o({h_j}^2)$$

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&= p(\boldsymbol{x}, t) + \frac{1}{4}\sum_{j=1}^{2}\Big({h_j}^2 p_{x_jx_j} + o({h_j}^2)\Big).
\end{aligned}$$

Canceling $p(\boldsymbol{x}, t)$ and dividing by τ yields:

$$p_t + o(1) = \frac{1}{4}\sum_{j=1}^{2}\left(\frac{h_j^{\,2}}{\tau}p_{x_j x_j} + o(\frac{h_j^2}{\tau})\right).$$

This time, to obtain nontrivial limit, we ask that:

$$\frac{h_j^{\,2}}{\tau} = 4k_j, \qquad k_j > 0, \quad j = 1, 2.$$

This results in a **diffusion equation**

$$\boxed{p_t = \sum_{j=1}^{2} k_j p_{x_j x_j} = k_1 p_{x_1 x_1} + k_2 p_{x_2 x_2}.}$$

Walks with drift

We can also set different probabilities in different directions. For example, if at time t, the particle is located at $\boldsymbol{x}$, then at time $t+\tau$ it is
at $\boldsymbol{x} + h_1 \boldsymbol{e_1}$ with probability p_1,
at $\boldsymbol{x} - h_1 \boldsymbol{e_1}$ with probability q_1,
at $\boldsymbol{x} + h_2 \boldsymbol{e_2}$, with probability p_2,
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with $p_1 + q_1 = \frac{1}{2}$ and $p_2 + q_2 = \frac{1}{2}$.

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Then:

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Using the Taylor formulas from before:

$$p(\boldsymbol{x}, t+\tau) = p(\boldsymbol{x}, t) + p_t(\boldsymbol{x}, t)\tau + o(\tau)$$

$$q_j\, p(\boldsymbol{x} + h_j\boldsymbol{e_j}, t) = q_j\, p(\boldsymbol{x}, t) + q_j\, p_{x_j}(\boldsymbol{x}, t) h_j + \frac{q_j}{2} p_{x_j x_j}(\boldsymbol{x}, t) {h_j}^2 + o({h_j}^2)$$

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... we get:

$$p_t(\boldsymbol{x}, t)\tau + o(\tau) = \sum_{j=1}^{2} \left(\frac{1}{4} p_{x_j x_j}(\boldsymbol{x}, t) {h_j}^2 + (q_j - p_j)\, p_{x_j}(\boldsymbol{x}, t) h_j + o({h_j}^2) \right)$$

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If, in addition to $\frac{{h_j}^2}{\tau} = 4k_j$, we have

$$\frac{q_j - p_j}{h_j} \to \beta_j \quad \text{and} \quad b_j = 4k_j\beta_j,$$

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$$\boxed{p_t = \sum_{j=1}^{2} k_j p_{x_jx_j} + \sum_{j=1}^{2} b_j p_{x_j}}$$

One can also assume that the particle loses mass at the constant rate γ. That is, from time t to time $t + \tau$, the following part of the particle disappears:

$$Q(\boldsymbol{x}, t) = \tau \gamma p(\boldsymbol{x}, t).$$

Walks with drift and reaction

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Therefore,

$$p(\boldsymbol{x}, t+\tau) = \sum_{j=1}^{2}\left[q_j\Big(p(\boldsymbol{x}+h_j\boldsymbol{e_j}, t) - Q(\boldsymbol{x}+h_j\boldsymbol{e_j}, t)\Big) + p_j\Big(p(\boldsymbol{x}-h_j\boldsymbol{e_j}, t) - Q(\boldsymbol{x}-h_j\boldsymbol{e_j}, t)\Big)\right].$$

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Note that:

$$\begin{aligned}\sum_{j=1}^{2}\Big(q_j\,Q(\boldsymbol{x}+h_j\boldsymbol{e_j},t)+p_jQ(\boldsymbol{x}-h_j\boldsymbol{e_j},t)\Big)&=Q(\boldsymbol{x},t)+\sum_{j=1}^{2}(q_j-p_j)h_jQ_x(\boldsymbol{x},t)+\ldots\\&=\tau\gamma p(\boldsymbol{x},t)+O(\tau h_j),\end{aligned}$$

Walks with drift and reaction

Therefore,

$$p_t(\boldsymbol{x},t)\tau + o(\tau) = \sum_{j=1}^{2}\left(\frac{1}{4}p_{x_jx_j}(\boldsymbol{x},t){h_j}^2 + (q_j - p_j)\,p_{x_j}(\boldsymbol{x},t)h_j + o({h_j}^2) - \tau\gamma p(\boldsymbol{x},t) + O(\tau h_j)\right)$$

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Assuming, as before, that $\frac{h_j^2}{\tau} = 4k_j$ and $\frac{q_j - p_j}{h_j} \to \beta_j$ and $b_j = 4k_j\beta_j$, we obtain a **drift-diffusion-reaction equation**:

$$\boxed{p_t = \sum_{j=1}^{2} k_j p_{x_jx_j} + \sum_{j=1}^{2} b_j p_{x_j} - \gamma p.}$$