1. From Random Movements to PDEs

1.1. Heat Equation.

1.1.1. 1D Random walk.

Consider the random walk of a particle along the real line. Let the rule of movement be: At each time step of size τ, the particle jumps to left or right with distance h equally likely, that is with probability 1/2. Now assume at $t=0$ the particle is at $x=x_0$. We are interested in getting the probability density of the location of the particle $u(x,t)$, that is, the probability of finding the particle inside the interval $[a,b]$ at time t is $\int_a^b u(x,t)\,\mathrm{d}x$, as the time/space steps $\tau, h \searrow 0$.

We can either

- Explicitly calculate this probability and then study the limit $\tau \searrow 0$, or
- Obtain a differential equation satisfied by studying the relation between $u(x,t)$ at an earlier and a later time.

We will take the 2nd approach here, and leave the first one as exercise.

Consider the probability of the particle reaching location x at time $t+\tau$. According to the rules of the motion, there are only two possibilities: The particle was at $x-h$ at time t, and jumped to the right; or the particle was at $x+h$ at time t and jumped to the left. As the location of the particle at time t and the direction of its next movement are independent, the first situation happens with probability $\frac{1}{2}\,u(x-h,t)$ while the second with $\frac{1}{2}\,u(x+h,t)$. Therefore

$$u(x,t+\tau)=\frac{1}{2}\,u(x-h,t)+\frac{1}{2}\,u(x+h,t). \tag{1.1}$$

Now we Taylor expand both sides at x,t:

$$\begin{aligned} u(x,t+\tau) &= u(x,t)+u_t(x,t)\,\tau+o(\tau); & (1.2)\\ u(x\pm h,t) &= u(x,t)\pm u_x(x,t)\,h+\frac{1}{2}\,u_{xx}(x,t)\,h^2+o(h^2). & (1.3)\end{aligned}$$

Substituting into (1.1) we have

$$u_t+o(1)=\frac{1}{2}\,\frac{h^2}{\tau}\,u_{xx}+o\left(\frac{h^2}{\tau}\right). \tag{1.4}$$

Now we see that nontrivial dynamics only happen when $\frac{h^2}{\tau}\longrightarrow 2\,D$ for some positive and finite D. Thus we reach the equation satisfied by p as

$$u_t=D\,u_{xx}. \tag{1.5}$$

We see that the initial condition should be

$$u(x,0)=\delta(x-x_0). \tag{1.6}$$

Now if we have $u(x,0)=u_0(x)$, that is we do not know the exact location of the particle at time $t=0$, but instead know its probability distribution, then the problem becomes

$$u_t=D\,u_{xx}, \qquad u(x,0)=u_0(x). \tag{1.7}$$

Remark 1.1. **(Fundamental solution)** Let us denote the solution to the problem

$$u_t=D\,u_{xx}, \qquad u(x,0)=\delta(x) \tag{1.8}$$

by $K(x,t)$. Then we can conclude, from the symmetries of the underlying random walk,

- The solution to
$$u_t=D\,u_{xx}, \qquad u(x,0)=\delta(x-y) \tag{1.9}$$
is $K(x-y,t)$.
- The solution to
$$u_t=D\,u_{xx}, \qquad u(x,0)=u_1\,\delta(x-y_1)+\cdots+u_n\,\delta(x-y_n) \tag{1.10}$$

is

$$u_1 K(x-y_1,t)+\cdots+u_n K(x-y_n,t). \tag{1.11}$$

- Now using the definition of, say, Riemann integration, we conclude

$$u_t = D\,u_{xx}, \qquad u(x,0)=u_0(x) \Longrightarrow u(x,t)=\int_{\mathbb{R}} K(x-y,t)\,u_0(y)\,\mathrm{d}y. \tag{1.12}$$

Thus we obtained a formula for the solution of the general heat equation.

1.1.2. Drift and boundaries.

Drift.

If we assign different probability to left and right movements, say p_L to left and p_R to right, still independent of previous movements of the particle, then following similar argument, we would reach

$$u_t + o(1) = \frac{1}{2}\frac{h^2}{\tau}u_{xx} + \frac{p_L - p_R}{\tau} h\,u_x + o\left(\frac{h^2}{\tau}\right). \tag{1.13}$$

Now assume

$$\frac{p_R - p_L}{\tau} h \longrightarrow c, \qquad \frac{h^2}{\tau} \longrightarrow 2\,D, \tag{1.14}$$

we reach

$$u_t + c\,u_x = D\,u_{xx}. \tag{1.15}$$

Remark 1.2. Let's ignore the "diffusion" term $D\,u_{xx}$ and consider the effect of the term $c\,u_x$. Intuitively, if $p_R > p_L$, then the particle has an overall tendency of moving right, characterized by the difference $p_R - p_L$. On the other hand, we know that the solution to the transport equation

$$u_t + c\,u_x = 0 \tag{1.16}$$

is $u(x,t) = u_0(x - c\,t)$. As $p_R > p_L \Longrightarrow c > 0$, this is consistent with our understanding from the underlying random walk.

Boundaries.

Let's consider a boundary at $x = L$. Recall that a particle has probability p_R moving to the right, $p_L = 1 - p_R$ to the left.

- Absorbing boundary. In this case whenever the particle goes beyond $x = L$, it disappears. This leads to

$$u(L, t+\tau) = p_R\,u(L-h, t). \tag{1.17}$$

  Taylor expansion gives

$$u(L,t) + O(\tau) = p_R\,[u(L,t) + O(h)] \tag{1.18}$$

  which leads to

$$u(L,t) = (1 - p_L)\,u(L,t) \Longrightarrow u(L,t) = 0 \tag{1.19}$$

  unless we have $p_L = 0$. Of course $p_L = 0$ should not be under consideration here since to obtain a heat equation with drift we need $p_R - p_L \longrightarrow 0$ as $h, \tau \longrightarrow 0$.

- Reflecting boundary. In this case whenever a particle tries to move beyond $x = L$, it is bounced back to $x = L$. So

$$u(L, t+\tau) = p_R\,u(L-h,t) + p_R\,u(L,t). \tag{1.20}$$

  Taylor expansion gives

$$u(L,t) + O(\tau) = p_R\,[u(L,t) + O(h)] + (1 - p_L)\,u(L,t) \tag{1.21}$$

  which reduces to

$$O(\tau) = (p_R - p_L)\,u(L,t) + O(h). \tag{1.22}$$

It is now clear that we need to expand to higher orders. Recalling $\tau \sim h^2$, we first try to expand to $O(h)$:

$$u(L,t)+O(\tau)=p_R\,[u(L,t)-u_x\,h+O(h^2)]+(1-p_L)\,u(L,t) \tag{1.23}$$

which leads to

$$O(\tau)=(p_R-p_L)\,u(L,t)-p_R\,u_x(L,t)\,h+O(h^2) \tag{1.24}$$

Therefore

$$\frac{p_R-p_L}{h}\,u(L,t)-p_R\,u_x(L,t)=0. \tag{1.25}$$

If we set

$$\frac{p_R-p_L}{\tau}\,h\longrightarrow c,\qquad \frac{h^2}{\tau}\longrightarrow 2\,D,\qquad p_R\longrightarrow\mu \tag{1.26}$$

we have

$$\frac{c}{2\,D}\,u(L,t)-\mu\,u_x(L,t)=0. \tag{1.27}$$

1.1.3. Is heat equation physical?.

Recall that our assumption is the particle jumps a distance of h for each time step τ. Thus its "speed" is h/τ. However we then let $h,\tau\searrow 0$ while keeping $\frac{h^2}{\tau}\longrightarrow 2\,D$. This clearly implies $h/\tau\rightarrow\infty$, that is the particle has "infinity" speed. This is not physical.

Exercises.

Exercise 1.1. Derive in detail the equation for random walk in the following general case: The probability of the particle at $(x,\,t)$ moving left, right, staying, and disappearing are $p_L(x,\,t)$, $p_R(x,\,t)$, $p_S(x,\,t)$ and $p_D(x,\,t)$. Assume the sum of these probabilities is 1. Note that as $h,\,\tau\rightarrow 0$, these probabilities need to satisfy certain relations (similar to $p_R-p_L\sim h$).

Exercise 1.2. Consider random walk along 2D grids, with probabilities $p_{\text{up}}(x,t), p_{\text{down}}(x,t), p_{\text{left}}(x,t), p_{\text{right}}(x,t)$. Assume the sum of these probabilities is 1. Derive the corresponding heat equation. Note that as $h,\tau\rightarrow 0$, these probabilities need to satisfy certain relations (similar to $p_R-p_L\sim h$).

Exercise 1.3. Design an underlying random walk rule which gives the equation

$$u_t=D\,u_{xx}+f(x,t),\qquad u(x,0)=u_0(x). \tag{1.28}$$

Then use it to explain the following Duhamel's principle:

Duhamel's principle. The solution to the above problem is given by

$$u(x,t)=U(x,t)+\int_0^t v(x,t;s)\,\mathrm{d}s \tag{1.29}$$

where $U(x,t)$ is the solution to

$$u_t=D u_{xx},\qquad u(x,0)=u_0(x) \tag{1.30}$$

and $v(x,t;s)$ (with $t\geqslant s$) solves

$$v_t=D v_{xx},\qquad v(x,s;s)=f(x,s). \tag{1.31}$$

Exercise 1.4. (Parabolic Scaling) Consider the heat equation

$$u_t=D\,u_{xx}. \tag{1.32}$$

Find a relation between $\lambda,\mu>0$ such that if $u(x,t)$ is a solution, $u(\lambda\,x,\mu\,t)$ is also a solution. Do you think there is a relation to the requirement $h^2\sim\tau$? Why?

References.

- Sandro Salsa, "Partial Differential Equations in Action: From Modelling to Theory", §2.4. Note that this book is available online at ualberta library.
- Erich Zauderer, "Partial Differential Equations of Applied Mathematics", 2ed, §1.1.

1.2. Wave Equations.

In the previous section we mentioned that one shortcoming is that the particle has infinite speed: The root of this problem is the following: The particle moves left or right *independent* of what it has been doing. Such abrupt change of direction leads to huge cancellation of the movement[1.1], consequently to obtain non-trivial movement we need h^2/τ to be nonzero, that is we need infinite speed to negate the cancellation.

From this it is clear that the way to fix this problem is to make the particle's movement *dependent* on its history. More specifically, we require the particle to have a certain probability to keep its direction.

Let $\alpha(x,t)$ be the probability of a particle being at the point x and arriving from left, while $\beta(x,t)$ be that from the right. That is α,β are probability density functions[1.2] of left and right-moving particles. Let $p, q = 1-p$ be probabilities of persisting and reversing the direction of movement. Thus we have

$$\alpha(x,t+\tau) = p\,\alpha(x-h,t) + q\,\beta(x-h,t) \tag{1.33}$$

$$\beta(x,t+\tau) = p\,\beta(x+h,t) + q\,\alpha(x+h,t) \tag{1.34}$$

Taylor expansion leads to (as we set $\tau\sim h$ this time, the h^2 term is not necessary)

$$\alpha + \alpha_t\,\tau + o(\tau) = p\,[\alpha - \alpha_x\,h + o(h)] + q\,[\beta - \beta_x\,h + o(h)] \tag{1.35}$$

$$\beta + \beta_t\,\tau + o(\tau) = p\,[\beta + \beta_x\,h + o(h)] + q\,[\alpha + \alpha_x\,h + o(h)]. \tag{1.36}$$

Thus

$$\alpha_t\,\tau + p\,h\,\alpha_x + q\,h\,\beta_x = -q\,\alpha + q\,\beta + o(\tau) + o(h) \tag{1.37}$$

$$\beta_t\,\tau - p\,h\,\beta_x - q\,h\,\alpha_x = +q\,\alpha - q\,\beta + o(\tau) + o(h) \tag{1.38}$$

We see that non-trivial dynamics arise when $q\sim\tau$. Thus we set $p = 1 - \lambda\,\tau + o(\tau)$, $q = \lambda\,\tau + o(\tau)$. Dividing the above equations by τ and let $h/\tau \longrightarrow \gamma$, we reach

$$\alpha_t + \gamma\,\alpha_x = -\lambda\,\alpha + \lambda\,\beta, \tag{1.39}$$

$$\beta_t - \gamma\,\beta_x = \lambda\,\alpha - \lambda\,\beta. \tag{1.40}$$

with initial condition

$$\alpha(x,0) = \beta(x,0) = \frac{1}{2}\,\delta(x) \tag{1.41}$$

when we have one particle moving left or right with equal probability, or

$$\alpha(x,0) = \alpha_0\,(x), \qquad \beta(x,0) = \beta_0(x) \tag{1.42}$$

in the general case.

Note that this is a special case of the so-called "linear hyperbolic system" which will be studied in a future section. In this special case, we can re-write (1.39–1.40) to a single equation:[1.3]

Set $u = \alpha + \beta, v = \alpha - \beta$. Adding and subtracting (1.39–1.40) we get

$$u_t + \gamma\,v_x = 0; \qquad v_t + \gamma\,u_x = -2\,\lambda\,v. \tag{1.43}$$

1.1. If the step size if h, then after n steps, the distance – variance of the random variable given by the sum of the steps – is only $\sqrt{n}$.

1.2. Note that rigorously speaking, α, β are not probability density functions since they are not normalized – $\int\ \alpha \neq 1$, $\int\ \beta \neq 1$.

1.3. Recall that in ODE, higher order linear ODEs can be re-written into a first order system.

Now differentiating the second equation by ∂_x we have

$$v_{tx} + \gamma u_{xx} = -2\lambda v_x. \tag{1.44}$$

Using the first equation we have

$$v_{tx} = -\gamma^{-1} u_{tt}; \qquad v_x = \gamma^{-1} u_t. \tag{1.45}$$

Thus we finally reach

$$u_{tt} - \gamma^2 u_{xx} + 2\lambda u_t = 0. \tag{1.46}$$

This is called the *telegrapher's equation*.

Also we see that there are two initial conditions: $u(x,0) = \alpha(x,0) + \beta(x,0)$, $v(x,0) = \alpha(x,0) - \beta(x,0)$. As $u_t = -\gamma v_x$, the initial conditions for the u equation should be

$$u(x,0) = \alpha_0 + \beta_0, \qquad u_t(x,0) = -\gamma [\alpha_{0x} - \beta_{0x}]. \tag{1.47}$$

Remark 1.3. The physical meaning of γ and λ.

- The meaning of $\gamma = h/\tau$ is quite clear: It is the speed of the microscopic movement of the particles.
- For λ, recall that we set

  $$p = 1 - \lambda\tau + o(\tau), \qquad q = \lambda\tau + o(\tau). \tag{1.48}$$

  Thus a smaller λ means a lower tendency to reverse the direction of the movement.

Remark 1.4. It is clear that when $\lambda = 0$ this reduces to the standard wave equation

$$u_{tt} - \gamma^2 u_{xx} = 0. \tag{1.49}$$

We know that its solution is given by

$$u(x,t) = F(x - \gamma t) + G(x + \gamma t). \tag{1.50}$$

The initial profile will travel at speed γ – recall that $\gamma = h/\tau$.

From the last remark we see that setting $\lambda = 0$ gives

$$p = 1 + o(\tau), \qquad q = o(\tau) \tag{1.51}$$

which essentially means the particles are moving deterministically: Those initial moving left will always move left, and those initially moving right will always moving right.

Remark 1.5. (Wave, Telegraph, Heat) As they are all based on random movement of a particle, clearly there should be relation between these equations. We already see the relation between telegraph equation and wave equation. Now we present two ways to obtain heat equation from telegraph equation.

- Large λ. The heat equation corresponds to the case where the reversing probability is $1/2$. Therefore we must have $\lambda \sim 1/\tau$. In this case the three terms of the equation

  $$u_{tt} - \gamma^2 u_{xx} + 2\lambda u_t = 0 \tag{1.52}$$

have sizes $1, \gamma^2, \lambda \sim 1/\tau$. To obtain nontrivial dynamics, at least two terms must be at the same largest size. Thus we must have $\gamma^2 \sim 1/\tau$ or $h^2 \sim \tau$. When this happens, the u_{tt} term becomes negligible and the equation becomes

$$2\,\lambda\,u_t - \gamma^2\,u_{xx} = 0, \tag{1.53}$$

essentially the heat equation.

- Long time dynamics.

  Let's consider what happens when t is very large. In that case instead of looking at the dynamics every τ, we can choose to study what happens every $\mathrm{T} = N\,\tau$. At each time step τ, the particle has probability $p = 1 - \lambda\,\tau + o(\tau)$ to stay in the same direction. Thus at each T the probability of keeping and reversing direction should be

$$p = (1 - \lambda\,\tau + o(\tau))^N, \qquad q = 1 - p. \tag{1.54}$$

  Taking $\tau \searrow 0$ (doesn't matter $N \nearrow \infty$ or not), we have

$$p \sim e^{-\lambda \mathrm{T}}, \qquad q = 1 - e^{\lambda \mathrm{T}}. \tag{1.55}$$

  On the other hand, the square of the new "spatial step length" should be the variance of $x_1 + \cdots + x_N$ which can be shown to be $H^2 = \frac{\gamma^2}{\lambda}\,\mathrm{T}$.

  We see that when we study the long time behavior of the dynamics, we reach the relation $H^2 \sim \mathrm{T}$ and thus should get heat equation.

Exercises.

Exercise 1.5. Design a random walk rule which leads to the equation

$$u_{tt} - \gamma^2\,u_{xx} + c\,u_x + 2\,\lambda\,u_t = 0. \tag{1.56}$$

Exercise 1.6. Consider the case when the probabilities of persistence and reversal are different for left moving particles and right moving particles. Let the superscript + denote probabilities regarding right moving particles and − denote probabilities regarding left moving particles. Write $p^{\pm}(x) = \sigma(x) - \lambda^{\pm}(x)\,\tau$, $q^{\pm}(x) = \lambda^{\pm}(x)\,\tau$ note that for probability $1 - \sigma$ the particle remains at the same location. Show that the resulting system is

$$\alpha_t + \gamma\,(\sigma\,\alpha)_x + \lambda^+\,\alpha - \lambda^-\,\beta = 0, \tag{1.57}$$

$$\beta_t - \gamma\,(\sigma\,\beta)_x - \lambda^+\,\alpha + \lambda^-\,\beta = 0. \tag{1.58}$$

Then reduce it to a single equation by assuming $\lambda^{\pm}(x) = \lambda \mp \sqrt{\lambda}\,\psi(x)$:

$$u_{tt} - \gamma^2\,[\sigma\,(\sigma\,u)_x]_x + 2\,\sqrt{\lambda}\,\gamma\,(\sigma\,\psi\,u)_x + 2\,\lambda\,u_t = 0 \tag{1.59}$$

Exercise 1.7. Consider the case $p, q > 0$ be fixed numbers, $p + q = 1$. Let the random walk of the particle be such that it has probability p of keeping the direction and q of reversing. What equation can you get form this random walk?

References.

- Erich Zauderer, "Partial Differential Equations of Applied Mathematics", 2ed, §1.2.

1.3. Laplace and Poisson Equations.

1.3.1. Laplace equation.

Consider the following problem.

> **Problem No.1.** A particle starts from an interior point of a rectangular[1.4] region A, we ask for the probability of it reaching a certain boundary point $(x_0, y_0) \in \partial A$ before reaching other points (put differently, one can say that the particle "exits" once it hits the boundary, then we are talking about the probability of a particle "exit" at (x_0, y_0)).

This leads to

$$u(x, y) = \frac{1}{4}\left[u(x+h, y) + u(x-h, y) + u(x, y+h) + u(x, y-h)\right], \qquad u(x, y) = \begin{cases} 1 & (x, y) = (x_0, y_0) \\ 0 & \text{otherwise} \end{cases}. \tag{1.60}$$

Taking Taylor expansion, then dividing both sides by h^2 and taking $h \searrow 0$, we easily obtain *Laplace's equation*.

$$u_{xx} + u_{yy} = 0. \tag{1.61}$$

However the boundary conditions is a bit sublte to determine. Naïvely one may simply copy

$$u(x, y) = \begin{cases} 1 & (x, y) = (x_0, y_0) \\ 0 & \text{otherwise} \end{cases}. \tag{1.62}$$

However this is not correct.

Recall our original setting: $u(x, y)$ is the probability of the particle starting at (x, y) exits at $(x_0, y_0) \in \partial A$ instead of other boundary points. Therefore $u(x, y)$ should be a probability density defined on ∂A. With this understanding, we see that the correct boundary condition is

$$u(x, y) = \delta_{\partial A}(x - x_0, y - y_0). \tag{1.63}$$

Here the subscript ∂A is the emphasize that the δ here is not the usual 2D δ function. Instead it is normalized by

$$\int_{\partial A} \delta_{\partial A}(x - x_0, y - y_0)\, \mathrm{d}s = 1. \tag{1.64}$$

Remark 1.6. As before, if we denote the the solution of this problem by $K(x, y; x_0, y_0)$. Then the solution to the problem

$$u_{xx} + u_{yy} = 0, \qquad u(x, y) = g(x, y) \text{ on } \partial A \tag{1.65}$$

is given by

$$u(x, y) = \int_{\partial A} K(x, y; x', y')\, g(x', y')\, \mathrm{d}s. \tag{1.66}$$

Note that $K(x, y; x_0, y_0)$ is **not** a function of $x - x_0, y - y_0$ only anymore!

More about the properties of K as well as how compute it will be discussed in Math438 (Green's functions).

1.3.2. Poisson equation.

> **Problem No.2.** Now we ask the probability of a particle starting at an interior point $(x, y) \in A$ and reaching another interior point $(\xi, \eta) \in A$ before reaching the boundary (and exit, never to return, let's say). Let this probability be represented by $w(x, y)$ (as it is in fact a function of four variables x, y, ξ, η, later we will denote it as $G(x, y; \xi, \eta)$).

1.4. This is an artifact of setting an underlying "grid".

This time the boundary condition is easy:

$$w(x, y) = 0 \qquad (x, y) \in \partial A. \tag{1.67}$$

For the equation, we have

$$w(x, y) = \frac{1}{4}\left[w(x+h, y) + w(x-h, y) + w(x, y+h) + w(x, y-h)\right] \tag{1.68}$$

when $(x, y) \neq (\xi, \eta)$ but

$$w(x, y) = 1 + \frac{1}{4}\left[w(x+h, y) + w(x-h, y) + w(x, y+h) + w(x, y-h)\right] \tag{1.69}$$

when $(x, y) = (\xi, \eta)$. Now there is a problem: What does it mean to have $w(x, y) > 1$? To resolve this issue, we have to remember that $w(x, y)$ is in fact a probability density function so the probability for the point (x, y) is in fact $w(x, y)\, h^2 = 1$. (Needs better explanation!)

Taking limit $h \searrow 0$ we have

$$w_{xx} + w_{yy} = -\delta(x - \xi, y - \eta). \tag{1.70}$$

with boundary condition $w = 0$.

Remark 1.7. Again, if we denote by $G(x, y; \xi, \eta)$ the solution to the above problem, then the solution to

$$u_{xx} + u_{yy} = -f(x, y), \qquad u(x, y) = 0 \qquad (x, y) \in \partial A \tag{1.71}$$

is given by

$$u(x, y) = \int_A G(x, y; \xi, \eta)\, f(\xi, \eta)\, \mathrm{d}\xi\, \mathrm{d}\eta. \tag{1.72}$$

This G is called the *Green's function* for the Poisson equation with Dirichlet boundary condition (that is $u = 0$ on boundary).

Another model that leads to Poisson equation is to consider the expected mean first passage time of a particle. If we let time step to be τ and assume the particle leaves the domain once it hits the boundary, then clearly we have boundary condition

$$u(x, y) = 0 \text{ on } \partial A \tag{1.73}$$

while inside the domain

$$u(x, y) = \tau + \frac{1}{4}\left[u(x-h, y) + u(x+h, y) + u(x, y-h) + u(x, y+h)\right]. \tag{1.74}$$

If we let $h^2/\tau = 2\,D$, taking $h \searrow 0$ gives

$$u_{xx} + u_{yy} = -2/D. \tag{1.75}$$

Exercises.

Exercise 1.8. Consider particle moving with probabilities (p_1, q_1 left/right; p_2/q_2 up/down)

$$p_i(x, y) = \frac{1}{4}\left[a_i(x, y) + b_i(x, y)\, h\right], \quad q_i(x, y) = \frac{1}{4}\left[a_i(x, y) - b_i(x, y)\, h\right]. \tag{1.76}$$

Show that for Problem No.1 we get

$$a_1\, u_{xx} + a_2\, u_{yy} + 2\, b_1\, u_x + 2\, b_2\, u_y = 0. \tag{1.77}$$

For Problem No. 2 we get

$$(a_1\, w)_{xx} + (a_2\, w)_{yy} - 2\,(b_1\, w)_x - 2\,(b_2\, w)_y = -\delta(x - \xi)\, \delta(y - \eta). \tag{1.78}$$

References.

- Erich Zauderer, "Partial Differential Equations of Applied Mathematics", 2ed, §1.3.

1.4. Problems.

1.4.1. Explicit formula of the fundamental solution.

- Note: You need to fill in all details necessary (to you). Basically you need to expand this into a section.

Recall that if $K(x,t)$ solves

$$K_t = D\,K_{xx}, \qquad K(x,0) = \delta(x) \tag{1.79}$$

then the solution to the general case

$$u_t = D\,u_{xx}, \qquad u(x,0) = u_0(x) \tag{1.80}$$

is given by

$$u(x,t) = \int K(x-y,t)\,u_0(y)\,\mathrm{d}y. \tag{1.81}$$

Now we try to figure out the formula of $K(x,t)$ through solving the underlying random walk problem directly.

Consider the random walk of a particle along the line with time/spatial steps τ, h and equal probability $1/2$ of moving left or right. We derive $K(x,t)$ through the following steps.

a) Fixing h,τ, the probability of the particular reaching $x = m\,h$ at $t = N\,\tau$ is

$$p_{h,\tau}(x,t) = \begin{cases} \frac{\binom{N}{k}}{2^N} & N+m \text{ even} \\ 0 & N+m \text{ odd} \end{cases}. \tag{1.82}$$

where $k = \frac{N+m}{2}$ and $\binom{N}{k} := \frac{N!}{k!\,(N-k)!}$.

b) Recall Stirling's formula

$$n! \sim \sqrt{2\,\pi\,n}\,(n/e)^n \tag{1.83}$$

which means

$$\lim_{n\to\infty} \frac{n!}{\sqrt{2\,\pi\,n}\,(n/e)^n} = 1. \tag{1.84}$$

We conclude that

$$p_{h,\tau}(x,t) \sim \frac{1}{\sqrt{2\,\pi}} \frac{\sqrt{N}}{\sqrt{(N+m)/2}\,\sqrt{(N-m)/2}} \frac{1}{\left(1-\frac{m^2}{N^2}\right)^{N/2}\left(1+\frac{m}{N}\right)^{m/2}\left(1-\frac{m}{N}\right)^{-m/2}}. \tag{1.85}$$

Explain what $\sim$ means here.

c) Fix (x,t) and the ration $h^2/\tau = 2\,D$. We have $N = \frac{2\,D\,t}{h^2}$, $m = \frac{x}{h}$. Taking $h \searrow 0$ we have

$$p_{h,\tau}(x,t) \sim \frac{1}{\sqrt{\pi\,D\,t}} \exp\left[-\frac{x^2}{4\,D\,t}\right] h. \tag{1.86}$$

Consequently (remember that $p = 0$ when $N+m$ is odd)

$$K(x,t) = \frac{1}{2\,\sqrt{\pi\,D\,t}} \exp\left[-\frac{x^2}{4\,D\,t}\right]. \tag{1.87}$$

d) Modify the above approach to obtain the fundamental solution for

$$u_t + c\,u_x = D\,u_{xx}. \tag{1.88}$$

1.4.2. Backward Kolmogorov equation.

Consider the random walk problem with left/right moving probabilities $p_L + p_R = 1$, and time/spatial steps τ, h. We consider the following problem:

If we know the particle is at x_0 at time $T > 0$, what are the probability distribution of this particle at time $t < T$?

Denote this solution by $u(x, t)$. Then since the particle only moves with step length h, we know that if a particle starts from x at time t reaches x_0 at time T, it must pass either $x - h$ or $x + h$ at time $t + \tau$. This leads to

$$u(x, t) = p_L\, u(x - h, t + \tau) + p_R\, u(x + h, t + \tau) \tag{1.89}$$

which gives

$$u_t + c\, u_x = -D\, u_{xx} \tag{1.90}$$

if we set $\frac{h^2}{\tau} \longrightarrow 2\,D$, $\frac{p_R - p_L}{\tau}\, h \longrightarrow c$.

Now consider the situation where the left/right moving probabilities are $p_L(x, t), p_R(x, t)$ depending on x and t. Derive the corresponding equation for $u(x, t)$ and compare with the forward Kolmogorov equation.

References.

- Erich Zauderer, "Partial Differential Equations of Applied Mathematics", 2ed, §1.1.

1.4.3. A more general framework.

A more general framework – any dimension, no grid – is as follows. Consider a "kernel" $k(x', x, t, \tau)$ which characterizes the probability of a particle at x at time t will reach x' at time $t+\tau$. Then the equation for the probability density function $u(\boldsymbol{x}, t)$ is

$$u_t = -(c\,u)_x + (d\,u)_{xx} \tag{1.91}$$

with

$$c(x,t) = \lim_{\tau\to 0} \frac{1}{\tau} \int_{-\infty}^{\infty} (x'-x)\, k(x', x, \tau, t)\, \mathrm{d}x' \tag{1.92}$$

$$d(x,t) = \lim_{\tau\to 0} \frac{1}{2\,\tau} \int_{-\infty}^{\infty} (x'-x)^2\, k(x', x, \tau, t)\, \mathrm{d}x' \tag{1.93}$$

One can show that the most basic case – time/spatial steps τ, h, with left/right probability p_L, p_R – corresponds to

$$k(x', x, \tau, t) = p_R\, \delta(x'-x-h) + p_L\, \delta(x'-x+h). \tag{1.94}$$

In higher dimension – for simplicity we present the 2D case here – we have

$$u(\boldsymbol{x}, t+\tau) = \int\!\!\int u(\boldsymbol{x}', t)\, k(\boldsymbol{x}', \boldsymbol{x}, \tau, t)\, \mathrm{d}\boldsymbol{x}' \tag{1.95}$$

which gives

$$u_t + \nabla\cdot[\boldsymbol{c}(\boldsymbol{x}, t)\, u] = \nabla\cdot\nabla\cdot[D(\boldsymbol{x}, t)\, u] \tag{1.96}$$

that is (let N be the dimension)

$$u_t + (c_1\, u)_x + (c_2\, u)_y = (D_{11}\, u)_{xx} + (D_{22}\, u)_{yy} + (D_{12} u + D_{21} u)_{xy}. \tag{1.97}$$

where

$$\boldsymbol{c} = \lim_{\tau\to 0} \frac{1}{\tau} \int (\boldsymbol{x}'-\boldsymbol{x})\, k(\boldsymbol{x}', \boldsymbol{x}, \tau, t)\, \mathrm{d}\boldsymbol{x}', \tag{1.98}$$

$$D = \lim_{\tau\to 0} \frac{1}{2\,\tau} \int [(\boldsymbol{x}'-\boldsymbol{x}) \otimes (\boldsymbol{x}'-\boldsymbol{x})]\, k(\boldsymbol{x}', \boldsymbol{x}, \tau, t)\, \mathrm{d}\boldsymbol{x}'. \tag{1.99}$$

Here the new symbols are defined as follows:

$$\boldsymbol{x} := (x, y); \qquad \boldsymbol{x}' := (x', y'); \qquad \mathrm{d}\boldsymbol{x}' := \mathrm{d}x'\,\mathrm{d}y'; \qquad \boldsymbol{x} \otimes \boldsymbol{y} := \begin{pmatrix} x_1\,y_1 & x_1\,y_2 \\ x_2\,y_1 & x_2\,y_2 \end{pmatrix}. \tag{1.100}$$

When we consider the x direction and the y direction are independent, then $D = d\,I = d\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and we reach

Taking directions into account.

If the particle simply moves along a particular direction with speed $\boldsymbol{c}(x, t)$, then we have

$$k = \delta(\boldsymbol{x} - \boldsymbol{x}' - \tau\,\boldsymbol{c}(x, t)). \tag{1.101}$$

Then we get

$$u_t = -\nabla \cdot (\boldsymbol{c}(x, t)\,u). \tag{1.102}$$

More often the particle's movement will be biased toward a direction $\hat{\phi}$ (for example think of the particle as a wandering animal and $\hat{\phi}$ points toward its den). In this case we have the following model:

$$k(\boldsymbol{x}', \boldsymbol{x}, \tau, t) = \frac{1}{\rho}\,f_\tau(\rho)\,K_\tau\big(\phi, \hat{\phi}\big) \tag{1.103}$$

where $\boldsymbol{x}' - \boldsymbol{x} = \begin{pmatrix} \rho\cos\phi \\ \rho\sin\phi \end{pmatrix}$ is the polar coordinate representation, $f_\tau(\rho)$ is a decreasing function modeling the size of the step – for example if the unit time step size is h then $f_\tau(\rho) = \delta(\rho - h)$. The factor $1/\rho$ is due to polar coordinate. The kernel $K_\tau\big(\phi, \hat{\phi}\big)$ is usually taken as

$$K_\tau\big(\phi, \hat{\phi}\big) = K\big(\phi - \hat{\phi}\big) \tag{1.104}$$

with $K(\theta)$ an even function taking maximum at $\theta = 0$. An example of $K\big(\phi, \hat{\phi}\big)$ is the *von Mises distribution*

$$K = \frac{1}{2\,\pi\,I_0(\kappa)} \exp\big[\kappa\cos\big(\phi - \hat{\phi}\big)\big]. \tag{1.105}$$

I_0 is modified Bessel function whose purpose is to make $\int_0^{2\pi} K\big(\phi, \hat{\phi}\big)\,\mathrm{d}\hat{\phi} = 1$.

Under such assumptions we can show that

$$\boldsymbol{c}(\boldsymbol{x}, t) // -\frac{\boldsymbol{x}}{|\boldsymbol{x}|} \tag{1.106}$$

that is $\boldsymbol{c}(\boldsymbol{x}, t)$ points toward the origin. We can also show that D is diagonal.

Reference.

- Paul R. Moorcroft, Mark A. Lewis, "Mechanistic Home Range Analysis", Chapters 2,3, Appendix E.

1.4.4. Correlated random walk.

Consider a particle moving randomly with time and spatial step sizes τ, h respectively. Let $p+q=1$ be the probability of this particle keeping and reversing its direction of movement.

We have seen that when we set $p=q=1/2$, we have to set $h^2 \sim \tau$ and reach heat equation; When we set $p=1-O(\tau)$ and $q=O(\tau)$, we have to set $h \sim \tau$ and reach telegrapher's (or wave if $O(\tau)$ becomes $o(\tau)$) equation. But why we have to set-up things this way? Also clearly there are all different situations in between, what happens then? In this subsection we try to understand these issues.

First recall the reason why in the first case we have to let $h/\tau \rightarrow \infty$. The reason is that when $p=q=1/2$, there is so much cancellation that if h/τ remains finite, or more precisely if $h^2 \ll \tau$, then as $\tau \longrightarrow 0$, the average distance between the particle and its starting location $\longrightarrow 0$ too, resulting no dynamics.

With this understood, we see that the key is to set the parameters such that the variance of

$$X_n := x_1 + \cdots + x_n \tag{1.107}$$

with x_i a random variable representing each step is finite – not 0, not ∞.

By symmetry we always have $E(X_n)=0$. So the variance is

$$E(X_n^2) = \sum_{i,j=1}^{n} E(x_i x_j) = n\,h^2 + 2 \sum_{i,j=1, i<j}^{n} E(x_i x_j). \tag{1.108}$$

To obtain the correlations $E(x_i x_j)$, we first consider $j=i+1$.

Set $\rho = p-q$. Then we have

$$E(x_{i+1}|\, x_i = \pm h) = \pm \rho\, h \tag{1.109}$$

Now one calculates

$$E(x_i x_{i+1}) = \rho\, h^2. \tag{1.110}$$

Let

$$P = \frac{1}{2} \begin{pmatrix} 1+\rho & 1-\rho \\ 1-\rho & 1+\rho \end{pmatrix} \tag{1.111}$$

be the transitional matrix which gives the probability each state of x_i to each of x_{i+1}.

We can show that the transitional matrix from x_i to x_{i+k} is P^k and consequently

$$E(x_{i+k}, x_i) = \rho^k. \tag{1.112}$$

Now we have

$$E(X_n^2) = h^2 \left[n + \frac{2\,n\,\rho}{2-\rho} - \frac{2\,\rho\,(1-\rho^n)}{(1-\rho)^n} \right]. \tag{1.113}$$

Requiring it to have a finite limit between 0 and ∞, we can obtain, for each relation $\tau \sim h^\alpha$, the relation between τ and ρ.

References.

- Erich Zauderer, "Partial Differential Equations of Applied Mathematics", 2ed, §1.3.