Lecture topics for 18306.

R. R. Rosales (MIT, Math. Dept., 2-337).   April 15, 2014

These are brief summaries of the 18.306 lectures. Further details can be found in the course web page notes, books, etc. These summaries will be updated from time to time. Check the date.

Contents

1 The heat/diffusion equation.

1.1 Random walks and Brownian motion in 1-D [S13].

For an alternative presentation of this topic, see the book by Salsa listed in the syllabus.

Consider a symmetric discrete random walk on the line, described by:

If the walker is at position x at time t, then at time $t+k$ it is at $x \pm h$, with probability $\frac{1}{2}$ each, (1.1)

where $k = \Delta t > 0$ and $h = \Delta x > 0$ are the discrete time and space steps, respectively. Hence the probability distribution function (pdf) for the process satisfies

$$p(x,\, t+k) = \frac{1}{2}\, p(x-h,\, t) + \frac{1}{2}\, p(x+h,\, t). \tag{1.2}$$

Note 1.1 *Strictly speaking (1.1) does not represent a single random walk, but infinitely many separate ones: one in each of the space-time grids* $\{x_m = x_0 + m\,h,\ t_n = t_0 + n\,k\}$, *where* $0 \le x_0 < h$ *and* $0 \le t_0 < k$. *Further: each choice of* k *and* h *produces a different set of walks. However, here we treat all these walks as a single one (with a single pdf) and justify it later — see remark 1.2.*

Note 1.2 *Note that (1.1) is a (rather coarse) simplification of the actual physics of real particles undergoing Brownian motion. For them the motion does not occur in steps of fixed length over fixed time intervals. A better model would be one in which the steps occur at random times, and have random lengths (the main approximation now being that we consider each jump as occurring instantaneously). However, as long as the jumps are independent, the details do not matter in the limit taken below — because of the Central Limit Theorem.*

Assume now that p in (1.2) is continuously differentiable (twice in time, thrice in space), write the equation in the form $p(x,\,t+k)-p(x,\,t) = \frac{1}{2}\left(p(x-h,\,t)+\frac{1}{2}p(x+h,\,t)-2\,p(x,\,t)\right)$, and expand in the limit $k, h \ll 1$. This yields

$$p_t = \frac{1}{2}\,\frac{h^2}{k}\,p_{x\,x} + O\left(\frac{h^3}{k},\,k\right). \tag{1.3}$$

If we now take the limit

$$h \downarrow 0 \quad \text{and} \quad h^2 = 2\,\nu\,k, \quad \text{where} \quad \nu > 0 \tag{1.4}$$

is a constant, we obtain the *diffusion equation* for p, with *diffusion coefficient* ν

$$p_t = \nu\,p_{x\,x}. \tag{1.5}$$

Note 1.3 *The limit in (1.4) is, of course, only an approximation in terms of the physics of Brownian motion. For example: consider the molecules in a gas. Then we interpret* h *and* k *as the mean distance and time between collisions. But then* $v = h/k$ *is related to the mean velocity of the molecules while in free flight between collisions. Clearly,* $v \neq \infty$, *as (1.4) implies — however, as long as it is large enough compared with the other scales in the problem,* $v \approx \infty$ *is acceptable.*

The particular situation where the walker position, say $x = 0$, is known at time $t = 0$ corresponds to the initial data, and solution,

$$p(x,\,0) = \delta(x) \quad \Longrightarrow \quad p = p_* = \frac{1}{\sqrt{4\,\pi\,\nu\,t}}\,\exp\left(-\frac{x^2}{4\,\nu\,t}\right). \tag{1.6}$$

Remark 1.1 Expected values. *The Fourier transform of the pdf can be used to easily compute expected values.*[1] *For example:*

$$P_*(\kappa,\,t) = \int_{-\infty}^{\infty} p_*(x,\,t)\,e^{i\,\kappa\,x}\,dx = \frac{1}{\sqrt{2\,\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}s^2 + i\,\kappa\,\sqrt{2\,\nu\,t}\,s}\,ds = \exp\left(-\kappa^2\,\nu\,t\right). \tag{1.7}$$

[1] It plays the same role, for stochastic variables, that the generating function plays for discrete random variables.

Hence

$$E(x) = \int_{-\infty}^{\infty} x\, p_*(x,\, t)\, dx = -i\, \partial_\kappa P_*(0,\, t) = 0 \tag{1.8}$$

and

$$E(x^2) = \int_{-\infty}^{\infty} x^2\, p_*(x,\, t)\, dx = -\partial_\kappa^2 P_*(0,\, t) = 2\,\nu\, t. \tag{1.9}$$

That is: in unit time the particle diffuses, on average, a distance $\sqrt{2\,\nu}$. ♣

Remark 1.2 Justification of the limit taken. *As follows from the points in note 1.1, the expansions leading to (1.3) are not quite justified. For example, assume that* $p_0 = p(x,\, 0)$ *is given at time* $t = 0$ *— with* p_0 *smooth. Then (1.2) defines* p *for all* $t = n\,k$*, but not values of* t *other than these. Furthermore, even for these values* p *is not just a function of* x *and* t*, as we assumed to get (1.3). That is:*

$$p(x,\, k) = \frac{1}{2}\, p_0(x+h) + \frac{1}{2}\, p_0(x-h), \quad p(x,\, 2\,k) = \frac{1}{4}\, p_0(x+2\,h) + \frac{1}{2}\, p_0(x) + \frac{1}{4}\, p_0(x-2\,h),$$

and so on. This means that, in general, it should be $p = p(x, t, h,\, k)$ *… thus one may ask: where are the partial derivatives*[2] *with respect to* h *and* k *in (1.3)?*

Rather than try to "fix" the derivation of (1.5) given by (1.3 – 1.4), we present here an independent justification — which, unfortunately, lacks the simplicity of (1.3 – 1.4). We start by writing the exact solution to (1.2) for the times $t_n = n\,k$*, given some initial data* $p_0 = p(x,\, 0)$*. This we can do by finding the normal modes*[3] *for the discrete-time equation*

$$p_{n+1}(x) = \frac{1}{2}\, p_n(x-h) + \frac{1}{2}\, p_n(x+h), \tag{1.10}$$

where $p_n(x) = p(x,\, t_n)$*. That is*
$$p_n(x) = \frac{1}{2\,\pi} \int_{-\infty}^{\infty} (\cos\omega\, h)^n\, e^{-i\,\omega\, x}\, P_0(\omega)\, d\,\omega, \tag{1.11}$$

where P_0 *is the Fourier transform of* p_0 *— which we assume is smooth enough to guarantee rapid decay of* P_0 *as* $|\omega| \to \infty$*. Next we consider the limit — note that this is the same as (1.4) —*

$$T > 0 \text{ fixed, with } k = \frac{T}{N}, \quad h = \sqrt{2\,\nu\, k}, \quad \text{and } N \to \infty. \tag{1.12}$$

Thus, for any $t \geq 0$ *fixed and bounded* ω

$$(\cos\omega\, h)^n = \left(1 - \frac{\nu}{n}\, t_n\, \omega^2 + O\left(\frac{\omega^4}{N^2}\right)\right)^n \quad \longrightarrow \quad \exp(-\nu\, \omega^2\, t), \tag{1.13}$$

where n *is the integer part of* $\frac{t}{T}\, N$ *(so that* $t_n \to t$*). In addition* $\left|(\cos\omega\, h)^n\, e^{-i\,\omega\, x}\, P_0(\omega)\right| \leq |P_0(\omega)|$*. It follows that*

$$p_n \quad \longrightarrow \quad \frac{1}{2\,\pi} \int_{-\infty}^{\infty} e^{-i\,\omega\, x - \nu\, \omega^2\, t}\, P_0(\omega)\, d\,\omega, \tag{1.14}$$

which is exactly the solution to (1.5) with the given initial data. ♣

[2] Even worse: how is p defined for $n\,k < t < (n+1)\,k$, in such a way that the result is smooth and satisfies (1.2)?

[3] The ansatz $p_n(x) = G^n\, \phi(x)$ leads to the **self-adjoint** eigenvalue problem $G\,\phi(x) = \frac{1}{2}\,\phi(x+h) + \frac{1}{2}\,\phi(x-h)$.

Remark 1.3 Useful integrals: $\displaystyle\int_{-\infty}^{\infty} e^{-x^2}\,dx = \sqrt{\pi}$ *and* $\displaystyle\int_{-\infty}^{\infty} e^{i\,k\,x-\frac{1}{2}\,x^2}\,dx = \sqrt{2\,\pi}\,e^{-\frac{1}{2}\,k^2}$.

Proof. The first integral follows because $\displaystyle\left(\int_{-\infty}^{\infty} e^{-x^2}\,dx\right) = \iint e^{-x^2-y^2}\,dx\,dy = \int_0^{2\,\pi} d\theta \int_0^{\infty} e^{-r^2} r\,dr = \pi.$

The second follows by moving the contour in the complex plane from $z = x$ to $z = i\,k + x$. ♣

Remark 1.4 Anomalous diffusion, *where* $(\Delta x)^2 = 2\,\nu\,\Delta t$ *in (1.4) is replaced by* $(\Delta x)^2 = 2\,\nu\,(\Delta t)^{\delta}$, *for some* $0 < \delta \neq 1$ *is also of interest in science. Sub-diffusive transport,* $0 < \delta < 1$, *corresponds to situations where the probability of large jumps by the walkers is relatively small. Super-diffusion,* $\delta > 1$, *correspond to Lévy flights, where the probability of large jumps by the walkers is large.*

Sub-diffusion examples: **1.** Charge carrier transport in amorphous semiconductors [1, 2, 3]. **2.** Nuclear Magnetic Resonance diffusometry on percolation structures [4, 5]. **3.** Motion of a bead in a polymer network [6].

Super-diffusion examples: **1.** Tracer particles in vortex arrays in a rotating flow [7]. **2.** Layered velocity fields [8], and Richardson diffusion [9, 10, 11].

Interesting, though a bit controversial, is the *Lévy flight foraging hypothesis*, which states that natural selection should lead to Lévy flights since these optimize search efficiencies [12, 13]. In this context, Lévy flights have been used to model the behavior of sharks, bumblebees, dear, albatross, etc. [14, 15, 16].

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Exercise 1: a non-Brownian motion random walk.[4] Replace (1.1) by

If the walker is at position x at time t, then at time $t+k$ it is at $x+n\,h$ with probability $\dfrac{\gamma}{1+n^2}$, where $n = 0,\, \pm 1,\, \pm 2,\, \dots$ and γ is the constant defined by: $\sum_n \frac{\gamma}{1+n^2} = 1$. (1.15)

Then (1.2) must be replaced by

$$\begin{aligned} p(x,\, t+k) &= \sum_{n=-\infty}^{\infty} \frac{\gamma}{1+n^2}\, p(x+n\,h,\, t) \\ &= \gamma\, p(x,\, t) + \sum_{n=1}^{\infty} \frac{\gamma}{1+n^2}\, \left(p(x+n\,h,\, t) + p(x-n\,h,\, t)\right) \\ &= p(x,\, t) + \sum_{n=1}^{\infty} \frac{\gamma}{1+n^2}\, \left(p(x+n\,h,\, t) + p(x-n\,h,\, t) - 2\,p(x,\, t)\right), \end{aligned} \tag{1.16}$$

where (to obtain the last line) we have used that the definition of γ is equivalent to $2\sum_1^\infty \frac{\gamma}{1+n^2} = 1-\gamma$. Finally, we re-write this last formula in the form

$$p(x,\, t+k) = p(x,\, t) + \sum_{n=1}^{\infty} \frac{\gamma}{n^2}\, \Phi_n + \sum_{n=1}^{\infty} \left(\frac{\gamma}{1+n^2} - \frac{\gamma}{n^2}\right)\, \Phi_n, \tag{1.17}$$

where $\boldsymbol{\Phi_n = p(x+n\,h,\, t) + p(x-n\,h,\, t) - 2\,p(x,\, t)}$.

Exercise task: *Consider the limit of equation (1.17) as $h,\, k \to 0$, and perform an analysis analogous to the one in (1.3–1.5)* — the equation that p satisfies in this case is very different from (1.5). *Hints:*

h1. The first task is to calculate the leading order terms, for h and k small, for the terms on the left and the right of the equal sign in (1.17). The left side is easy; for the right side, see h3.

h2. Once h1 is done, a relationship between h and k, analogous (but not the same) as the one in (1.4) must be imposed, so that a non-trivial limit results.

h3. To compute the leading order terms for the right hand side in (1.17), note that: (i) Multiplication of the numerator and denominator of the first sum by h^2 leads to a form whose limit you should be able to write as an integral; (ii) Assume that p is twice continuously differentiable in x, with a bounded second derivative — say $|p_{xx}| \le C_2$. Then

$$|\Phi_n| = \left| \int_0^{n\,h} ds_1 \int_{-n\,h}^{0} p_{xx}(x+s_1+s_2,\, t)\, ds_2 \right| \le C_2\, n^2\, h^2. \tag{1.18}$$

This can be used to show that the second sum in (1.17) is $O(h^2)$.

[4] This is an example of a Lévy flight.

1.2 Simple stochastic ode and Fokker Planck equation.

We now consider a generalization of the situation in § 1.1, where the walker, in addition to the Brownian motion random walk, is subject to some external influence. Specifically, consider the 1-D stochastic ode

$$\dot{x} = g(x,\, t) + w, \tag{1.19}$$

where w stands for *white noise.*

Physical motivation. Imagine a particle immersed in a fluid, moving under the influence of a force f. If the induced flow is laminar, then the equation of motion is $\boldsymbol{m\,\ddot{x} + b\,\dot{x} = f(x,\, t)}$, where m is the mass of the particle and b is the damping coefficient due to the fluid drag. In the drag dominated limit,† this can be simplified to $\boldsymbol{\dot{x} = g}$, where $g = f/b$. If, in addition, the particle mass is small enough, it will also experience brownian motion due to the momentum transfers from impacts with the liquid's molecules — this is the white noise in (1.19).

† Note that, for small enough particles, drag is always dominant.

Let now $\boldsymbol{p = p(x,\, t)}$ be the pdf (probability distribution function) for the particle position. Using conservation of probability it follows that

$$\int_a^b p(x,\, t+k)\, dx = \int_{a-g(a,\,t)\,k}^{b-g(b,\,t)\,k} \frac{1}{2}\left(p(x-h,\, t) + p(x+h,\, t)\right)\, dx \tag{1.20}$$

for any constants $a < b$, where we make the assumption in (1.1) for the Brownian motion, and assume that k is "very small".[5] Split the integral on the right hand side of this equation in three pieces $\int_{a-g(a,\,t)\,k}^{a} + \int_a^b + \int_b^{b-g(b,\,t)\,k}$, and expand everything for h and k small. This yields

$$k\int_a^b p_t(x,\, t)\, dx + O(k^2) = k\, g(a,\, t)\, p(a,\, t) + \frac{h^2}{2}\int_a^b p_{xx}(x,\, t)\, dx - k\, g(b,\, t)\, p(b,\, t) + O(k^2,\, k\, h^2,\, h^4).$$

Hence

$$\int_a^b p_t(x,\, t)\, dx = -\int_a^b \left(g(x,\, t)\, p(x,\, t)\right)_x\, dx + \frac{h^2}{2\,k}\int_a^b p_{xx}(x,\, t)\, dx + O(k,\, h^2,\, \frac{h^4}{k}). \tag{1.21}$$

Taking now the same limit as in (1.3), we obtain

$$\int_a^b p_t\, dx = -\int_a^b (g\, p)_x\, dx + \nu\int_a^b p_{xx}\, dx. \tag{1.22}$$

Since this must be true for all $a < b$, it follows that

$$\boldsymbol{p_t + (g\, p)_x = \nu\, p_{xx}.} \tag{1.23}$$

This is the **Fokker-Planck equation** corresponding to (1.19).

Remark 1.5 *Note that here, as in (1.2 – 1.5), we have again operated as if p in (1.20) was smooth and independent of k and h.* ♣

[5] So that we can approximate the flow by $\dot{x} = g$ via $x(t-k) = x(t) - g(x,\, t)\, k$.

1.3 Brownian motion and Fick's law.

Here we do things a bit more mathematically rigorous than in § 1.2, without involving discrete time and space steps, at the price of loosing a bit of the physical intuition.

We **define a Brownian motion in 1-D** as a process where the probability, $P = P(\mu,\, t)$, of a jump (in the position of a particle) of magnitude μ over a time interval $t > 0$ scales with $\sqrt{t}$, is even in μ, and decays sufficiently fast as $\mu \to \infty$. Specifically, we will assume that [6]

$$P(\mu,\, t) = \rho\left(\frac{\mu}{\sqrt{t}}\right)\frac{d\mu}{\sqrt{t}}, \tag{1.24}$$

where $\rho \geq 0$ is even and integrable, with

$$\int_{-\infty}^{\infty} \rho(s)\, ds = 1 \quad \text{and} \quad \nu = \frac{1}{2}\int_{-\infty}^{\infty} s^2\, \rho(s)\, ds < \infty. \tag{1.25}$$

Remark 1.6 ***Why these conditions? What do they mean?***

1. *The scaling in (1.24) can be "motivated" by the limit in (1.3 – 1.5). Scaling space and time via the relationship in (1.4) leads to a meaningful limit as $k \to 0$. Any other choice, in the context of (1.3), leads to a trivial limit — i.e.: $p_t = 0$ if $h^2 \ll k$, or $p_{xx} = 0$ if $h^2 \gg k$.*
2. *The conditions $\rho \geq 0$ and $\int_{-\infty}^{\infty} \rho(s)\, ds = 1$ follow because P is a probability.*
3. *That ρ be even is a symmetry statement. Jumps to the left and to the right are equally likely.*
4. *$\int_{-\infty}^{\infty} s^2\, \rho(s)\, ds < \infty$ is a statement about the likelihood of large jumps: the probability of a large jump vanishes as the size of the jump grows, fast enough to make this integral exist.*

Conditions 1, 3, and 4 are modeling choices. When applied to any particular physical situation, these choices may or may not be good — this has to be checked (do not blindly apply mathematics to a problem and expect magic; "garbage in – garbage out" is something you must always be wary of). These are good choices for modeling the physics of Brownian motion. However: **other types of random walks arise. In particular ones where large jumps are not as rare as for Brownian motion, and violate 4 — then a scaling different from the one in 1 is needed.** It is also possible to have **biassed** random walks, with ρ not even. ♣

Assume now a particle position pdf at time $t = 0$ given by $p_0(x)$, which we assume bounded and continuously differentiable.[7] Let us now compute $N(t)$, defined by

$$N(t) = \int_0^{\infty} p(x,\, t)\, dx - \int_0^{\infty} p_0(x)\, dx, \tag{1.26}$$

where p **is the pdf for the particle position at a time $t > 0$**. Clearly

$$N(t) = \int_0^{\infty} \left(p_0(-x) - p_0(x)\right) \underbrace{\left(\int_x^{\infty} \rho\left(\frac{\mu}{\sqrt{t}}\right)\frac{d\mu}{\sqrt{t}}\right)}_{I} dx, \tag{1.27}$$

[6] Note that $P(\mu,\, 0) = \delta(\mu)\, d\mu$, since (for any test function) $\int P(\mu,\, t)\, \psi(\mu) = \int \rho(s)\, \psi\left(s\sqrt{t}\right)\, ds$.

[7] These are "technical" conditions, needed to justify the manipulations that follow.

where I is both the probability of either a jump of magnitude larger than x (thus to the right of the origin from $-x$), or smaller than $-x$ (thus to the left of the origin from x). Define

$$\phi(x) = \int_0^x (p_0(s) - p_0(-s))\, ds = p_0'(0)\, x^2 + o(x^2), \tag{1.28}$$

so that

$$N(t) = -\int_0^\infty \phi(x)\, \rho\left(\frac{x}{\sqrt{t}}\right) \frac{dx}{\sqrt{t}} = -\int_0^\infty \phi\left(s\sqrt{t}\right)\, \rho(s)\, ds. \tag{1.29}$$

Hence

$$\dot{N} = -\frac{1}{2\sqrt{t}} \int_0^\infty \phi'\left(s\sqrt{t}\right)\, \rho(s)\, s\, ds = -\frac{1}{2\sqrt{t}} \int_0^\infty \left(2\, p_0'(0)\, s\sqrt{t} + o\left(s\sqrt{t}\right)\right)\, \rho(s)\, s\, ds. \tag{1.30}$$

It follows that

$$\dot{N}(0) = -p_0'(0) \int_0^\infty \rho(s)\, s^2\, ds = -\nu\, p_0'(0). \tag{1.31}$$

The same calculation can be carried at any time and at any position, which shows that (given the definition of N)

$$\textbf{The Brownian motion's probability flux satisfies Fick's law: } \boldsymbol{\mathcal{F}_b = -\nu\, p_x}. \tag{1.32}$$

In particular, using the conservation of probability

$$p_t = \nu\, p_{xx}. \tag{1.33}$$

Using (1.32) we *can now give meaning to the notion of an ode with a white noise forcing.* In particular, (1.33) corresponds to the simplest example of pure brownian motion, which we write in the form

$$\frac{db}{dt} = w = \text{white noise}, \tag{1.34}$$

where $b = b(t)$ is the trajectory of a particle executing a brownian motion, as defined above. Note that here we *extend the meaning of the derivative notation $\dot{b} = db/dt$ beyond its standard calculus meaning,* since:

i Strictly speaking, there is no single trajectory, but rather a whole (very large) family of them, which occur with probability as described by the pdf p in (1.26 – 1.33).

ii It can be shown that, with probability 1, the members of the family in (i) are no-where differentiable. Thus $\dot{b}$ does not exist in the classical sense, and must be given a meaning, as done here: $\dot{b} = w$ is the "thing" that produces the probability flux in (1.32) — see (iii).

iii Consider a "regular" deterministic ode

$$\frac{dx}{dt} = f(x,\, t), \tag{1.35}$$

where f is some given function. If the initial data for this equation are random, then the solution will also be random — but only because the data is not known precisely. In this case the pdf, $p = p(x, t)$ for the solution satisfies

$$p_t + (f\,p)_x = 0. \tag{1.36}$$

Thus a "classical" derivative can be associated with a probability flux .... $\boldsymbol{\mathcal{F}_c = f\,p}$, which corresponds to simply advecting the pdf at speed f. The definition above generalizes this to other types of fluxes; in particular, note that: $\mathcal{F}_c$ *does not depend on derivatives of* p*, while the white noise flux does.*

Other examples of ode with white noise forcing are given further below.

Exercise 1:* *deterministic flux. .... Show that (1.36) applies.

Example 1.1 *Consider the stochastic ode in (1.19)*

$$\dot{x} = g(x,\,t) + w. \tag{1.37}$$

We interpret this equation as meaning that the flux of probability by (1.37) is given by the deterministic probability flux $\mathcal{F}_d = g\,p$ *plus the Brownian flux* $\mathcal{F}_b$*. Hence the associated pdf satisfies the Fokker-Planck equation (1.23)*

$$p_t + (g\,p)_x = \nu\,p_{xx}. \tag{1.38}$$

Example 1.2 *Consider now a (brownian) random walker for which inertia is important. Then both the velocity* v *and the position* x *are subject to random variations.*[8] *A simple model for this is given by*

$$\dot{x} = v + w_1 \quad \textit{and} \quad \dot{v} + b\,v = f(x,\,t) + w_2, \tag{1.39}$$

where w_1 *and* w_2 *are white noise,* b *is the drag coefficient,* f *is the applied force, and we have set the particle mass to one, for simplicity.*
In this case the pdf is a function of both x *and* v*,* $p = p(x,\,v,\,t)$*, and we interpret the equations as meaning that the flux of probability is given by the deterministic probability fluxes for* x *and* v*, plus the corresponding Brownian fluxes. That is*

$$\mathcal{F}^x = v\,p - \nu_1\,p_x \quad \textit{and} \quad \mathcal{F}^v = -b\,v\,p + f\,p - \nu_2\,p_v. \tag{1.40}$$

Conservation of probability then yields $p_t + (\mathcal{F}^x)_x + (\mathcal{F}^v)_v = 0$*. That is*

$$p_t + v\,p_x + (f\,p - b\,v\,p)_v = \nu_1\,p_{xx} + \nu_2\,p_{vv}. \tag{1.41}$$

[8] For the drag dominated walker in (1.24), after each impact from a liquid molecule, the particle velocity is reset to the equilibrium value $\dot{x} = g$ by the drag. By contrast, when inertia matters, the velocity changes are cumulative.

1.3.1 First order phase transition (example).

Consider a small particle in a potential force field, in the drag dominated limit, subject to Brownian motion (in 1-D). Hence

$$\dot{x} = g + w, \quad \text{where} \quad g = -V'(x), \tag{1.42}$$

and V is the potential. It follows that the pdf satisfies the equation

$$p_t = \nu\, p_{xx} + (V'\, p)_x = \mathcal{L}\, p, \tag{1.43}$$

where the operator $\mathcal{L}$ is defined by the formula. We will also assume that V is at least C^2, and that

$$V(x) \to \infty \text{ as } |x| \to \infty. \tag{1.44}$$

It can be shown that *there exists a weight function* $\boldsymbol{\sigma = \sigma(x) > 0}$ *such that,* with the scalar product [9]

$$\langle \psi_1,\, \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_1(x)^*\, \psi_2(x)\, \sigma(x)\, dx, \tag{1.45}$$

the following applies

a. The operator $\mathcal{L}$ is self-adjoint $\qquad \langle \psi_1,\, \mathcal{L}\,\psi_2 \rangle = \langle \mathcal{L}\,\psi_1,\, \psi_2 \rangle. \qquad (1.46)$

b. The operator $\mathcal{L}$ is negative semi-definite, with

$$\langle \psi,\, \mathcal{L}\,\psi \rangle = -\nu \int_{-\infty}^{\infty} \frac{|(\sigma\,\psi)'|^2}{\sigma}\, dx \leq 0. \tag{1.47}$$

In fact, note that $\langle \psi,\, \mathcal{L}\,\psi \rangle < 0$, except when $\psi \propto \sigma^{-1}$ — which turns out to be the eigenfunction corresponding to the eigenvalue zero.

If V grows sufficiently fast as $|x| \to \infty$ — see (1.44) — eigenvalues for $\mathcal{L}$ are all discrete:[10] $\lambda_0 = 0 > \lambda_1 > \lambda_2 > \lambda_3 \ldots$, so that the solution to (1.43) has the form

$$p = a_0\, \phi_0 + \sum_{1}^{\infty} a_n\, \phi_n\, e^{\lambda_n\, t}, \tag{1.48}$$

with coefficients $a_n = \langle \phi_n,\, p_0 \rangle$, where the eigenfunctions are a complete orthonormal set. In particular, as $t \to \infty$,

$$\boldsymbol{p \to a_0\, \phi_0}. \tag{1.49}$$

It is easy to see that the zero eigenfunction is

$$\boldsymbol{\phi_0 = \gamma\, e^{-\frac{1}{\nu}\, V}}, \tag{1.50}$$

where γ is a normalization constant. It follows that,

> *as $t \to \infty$, the most likely*[11] *position for the particle occurs at the location x_m where V achieves its absolute minimum.*

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[9] The * denotes complex conjugate.

[10] We will not show this here.

[11] Overwhelmingly so if ν is small.

In particular, if V has a parameter in it (say r) such that, as r crosses some critical value r_c there is a change in the absolute minimum [12] (from x_{m1} to x_{m2}), then the behavior of the particle changes abruptly, and it switches from being near x_{m1} to being near x_{m2}. This is an *example of a first order phase transition.*

Note the difference with the deterministic case. If w is not present in (1.42), then any local minimum of V provides a stable equilibrium point. In the presence of noise, only an absolute minimum is stable. Other minimums are, at best (if the value of V there is not too different from the global minimum) meta-stable.

***Exercise 2:* weight function and phase transition.**

Find σ and show that (1.46–1.47) apply, and that the zero eigenfunction ϕ_0 is proportional to σ^{-1}. *Hint. To find σ compute $J = \langle \psi_1, \mathcal{L}\,\psi_2 \rangle - \langle \mathcal{L}\,\psi_1, \psi_2 \rangle$ for an arbitrary choice of σ, moving all the derivatives "out" of ψ_2 by using integration by parts. Setting $J = 0$ will then give you an equation for σ. Once you have σ, (1.47) follows by a bit of algebra and integration by parts.*

Furthermore, consider the case where $V = \frac{2}{3}\,r\,x^3 - \frac{1}{2}\,x^2 + \frac{1}{4}\,x^4.$
Compute r_c, as well as the position and values of V at the local maximums and minimums.

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2 More on the heat/diffusion equation.

2.1 Duhamel's principle [S16].

For an alternative presentation of this topic, see the book by Salsa listed in the syllabus.

Consider a nonhomogeneous (forced) linear problem of the form

$$Y_t = \mathcal{L}\,Y + F \quad \text{for} \quad t > 0, \quad \text{with initial data} \quad Y(0) = 0. \tag{2.1}$$

Here $\mathcal{L}$ is a (time independent) linear operator in some vector space (see note 2.1), where the forcing function $F = F(t)$ and the solution $Y = Y(t)$ take values in. Define now $W = W(t,\, s)$ by

$$W_t = \mathcal{L}\,W \quad \text{for} \quad t > s, \quad \text{with initial data} \quad W(s,\, s) = F(s). \tag{2.2}$$

Then **the solution to (2.1) is**

$$\boldsymbol{Y(t) = \int_0^t W(t,\, s)\, ds}. \tag{2.3}$$

Proof. Take the time derivative of (2.3), and assume that $\mathcal{L}$ commutes with the integration in s.

[12] Example: at two local minimums there is a switch from $V(x_{m1}) < V(x_{m2})$ to $V(x_{m1}) > V(x_{m2})$.

Note 2.1 *The vector space to which the solutions to (2.1) belong may be finite dimensional, in which case (2.1) is an ode, or not. When the space is not finite dimensional (e.g.: example 2.1) we will assume that the space (and the operator $\mathcal{L}$) have sufficient extra structure to guarantee that the various initial value problems above are all well-posed.* ♣

Example 2.1 *Consider the forced heat equation problem (here $\nu > 0$ is a constant)*

$$u_t - \nu\, u_{x\,x} = f(x,\, t) \quad \textit{for} \;\; t > 0 \;\; \textit{and} \;\; -\infty < x < \infty, \quad \textit{with initial data} \;\; u(x,\, 0) = 0. \tag{2.4}$$

Then $\boldsymbol{u(x,\, t) = \int_0^t w(x,\, t,\, s)\, ds,}$ *where w is defined by*

$$w_t - \nu\, w_{x\,x} = 0 \quad \textit{for} \;\; t > s \;\; \textit{and} \;\; -\infty < x < \infty, \quad \textit{with initial data} \;\; w(x,\, s,\, s) = f(x,\, s). \tag{2.5}$$

In particular, using the fundamental solution for the heat equation

$$G_f(x,\, t) = \frac{1}{\sqrt{4\,\pi\,\nu\,t}}\, \exp\left(-\frac{x^2}{4\,\nu\,t}\right) \tag{2.6}$$

we can write

$$u = \int_0^t ds \int_{-\infty}^{\infty} dy\; G_f(x - y,\, t - s)\, f(y,\, s). \tag{2.7}$$

This last formula shows that **the Green function for the problem in (2.4) is**

$$\boldsymbol{G_*(x,\, t) = 0} \;\; \textit{for} \;\; \boldsymbol{t < s} \quad \textit{and} \quad \boldsymbol{G_*(x,\, t) = G_f(x - y,\, t - s)} \;\; \textit{for} \;\; \boldsymbol{t > s.} \tag{2.8}$$

That is $\boldsymbol{u = G_*}$ satisfies

$$\boldsymbol{u_t - \nu\, u_{x\,x} = \delta(x - y)\, \delta(t - s)} \quad \textit{for} \;\; \boldsymbol{t > 0} \;\; \textit{and} \;\; \boldsymbol{-\infty < x < \infty,} \tag{2.9}$$

with initial data $\boldsymbol{u(x,\, 0) = 0}$ — where $\boldsymbol{s > 0}$ and $\boldsymbol{-\infty < y < \infty}$ are constants.

*Next we show that **(2.8) is, precisely, Duhamel's principle (2.3) applied to (2.9).***

In this case Duhamel's principle says that

$$\boldsymbol{G_*(x,\, t) = \int_0^t w(x,\, t,\, \tau)\, d\tau,} \tag{2.10}$$

with w is defined by

$$w_t - \nu\, w_{x\,x} = 0 \quad \textit{for} \;\; t > \tau \;\; \textit{and} \;\; -\infty < x < \infty, \;\; \textit{with} \;\; w(x,\, \tau,\, \tau) = \delta(x - y)\, \delta(\tau - s). \tag{2.11}$$

The solution to this is

$$w = G_f(x - y,\, t - \tau)\, \delta(\tau - s), \tag{2.12}$$

which upon substitution into (2.10) yields (2.8).

However, (2.12) involves a Dirac delta in the solution, so a bit of caution is needed.[13] *The approach in (2.4 – 2.7) avoids these difficulties.*

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[13] Before taking it seriously, we should check it by formulating everything in terms of test functions. And we also ought to check the proof of Duhamel's principle in this context. Turns out everything checks, but we have not done it here.

2.2 Tychonov's example [S17].

For an alternative presentation of this topic, see the book by Salsa listed in the syllabus.

It is a bit surprising that, unless extra restrictions on the solutions are imposed, the initial value problem for the heat equation on unbounded domains does not have a unique solution. Either of the following two restrictions is enough to guarantee uniqueness

1. The solution is **non-negative.**

2. There are constants a and b such that $|\boldsymbol{T}| \leq \boldsymbol{a\, e^{b\,x^2}}$. (2.13)

A proof of these results is beyond the scope of this course. Item **2** is a corollary of the:

Global maximum principle:

If $u_t - u_{x\,x} \leq 0$ for $t > 0$ and $-\infty < x < \infty$, and $u \leq a\,e^{b\,x^2}$ for some constants a and b, then the supremum of u occurs for $t = 0$. (2.14)

Tychonov's solution provides an (in fact, many) examples showing that uniqueness is lost if either **1** or **2** fails.[14] The solution is given by

$$T = \sum_{0}^{\infty} \frac{1}{(2\,n)!}\, x^{2\,n}\, h^{(n)}(t), \tag{2.15}$$

where $h^{(n)}$ is the n^{th} derivative of $\boldsymbol{h(t) = \exp(-1/t^p)}$, for some $p > 1$. It can be shown that

A. $\boldsymbol{T}$, as defined by (2.15), satisfies $\boldsymbol{T_t = T_{x\,x}}$. This is easy to do by differentiating the series term by term — justified because the series, and the series of term-by-term derivatives, converge absolutely and uniformly in any set where, for some constant M, $x^2 \leq M\,t$ [see (2.18)].

B. $\boldsymbol{T}$, as defined by (2.15), satisfies $\boldsymbol{T(x, 0) = 0}$, because $h^{(n)}(0) = 0$ for all n. In fact, it can be shown that all the partial derivatives of $\boldsymbol{T}$ vanish for $\boldsymbol{t = 0}$! On the other hand $\boldsymbol{T_{2nx}(0,\, t) = h^{(n)}(t) \neq 0}$. This shows that uniqueness for the initial value problem for the heat equation in the line fails if no restrictions are imposed — any linear combination of solutions of the form in (2.15) can be added to the solution.

The main fact that allows a proof convergence is: There exists constants $\boldsymbol{0 < \mu,\ K < 1}$ such that

$$\left|h^{(n)}(t)\right| \leq \frac{n!}{(\mu\,t)^n}\, \exp\left(-\frac{K}{t^p}\right) \quad \text{for } \textbf{all} \quad t > 0 \quad \text{and } \textbf{all} \quad n = 0,\, 1,\, 2, \dots \tag{2.16}$$

This is not too hard to show using the following consequence of Cauchy's theorem (applied to the function e^{-1/z^p}, analytic for $\text{Re}(z) > 0$)

$$h^{(n)}(t) = \frac{n!}{2\,\pi\,i} \int_{\Gamma} \frac{e^{-1/z^p}}{(z-t)^{n+1}}\, dz \quad \text{for any} \quad t > 0 \ \text{ and } \ 0 < \mu < 1, \tag{2.17}$$

[14] Clearly, a situation with lack of uniqueness must violate both **1** and **2**.

where Γ is a circle of radius $r = \mu\, t$, centered at $z = t$, tracked in the counter-clockwise direction — i.e.: $z = t + \mu\, t\, e^{i\,\phi}$, with $-\pi \le \phi \le \pi$.

From (2.16) it follows that

$$\sum_0^\infty \left| \frac{1}{(2\,n)!}\, x^{2\,n}\, h^{(n)}(t) \right| \;\le\; \sum_0^\infty \frac{n!}{(2\,n)!}\, \frac{x^{2\,n}}{(\mu\, t)^n}\, \exp\left(-\frac{K}{t^p}\right)$$
$$\le\; \sum_0^\infty \frac{1}{n!}\, \frac{x^{2\,n}}{(2\,\mu\, t)^n}\, \exp\left(-\frac{K}{t^p}\right) \;=\; \exp\left(\frac{x^2}{2\,\mu\, t} - \frac{K}{t^p}\right). \tag{2.18}$$

which shows the absolute convergence of the series for T. Similar calculations can be done for the series of term-by-term derivatives of T.

2.3 Nonlinear diffusion equation and finite propagation speed [S18].

For an alternative presentation of this topic, see the book by Salsa listed in the syllabus.

Porous media equation.

Consider a gas flowing through a porous media, with density ρ and flow velocity $\vec{u}$. Then the **conservation of mass** gives the equation

$$\rho_t + \mathrm{div}(\rho\, \vec{u}) = 0. \tag{2.19}$$

On the other hand, Darcy's law for porous media says that

$$\vec{u} = -\frac{\mu}{\nu}\, \mathrm{grad}\, p, \tag{2.20}$$

where $0 < \mu =$ permeability of the media, $0 < \nu =$ gas viscosity, and $p =$ gas pressure. Finally, if the flow is adiabatic, the **equation of state $\boldsymbol{p = p(\rho)}$** follows (e.g.: $p \propto \rho^\gamma$). Putting this all together yields the nonlinear diffusion equation

$$\rho_t = \mathrm{div}\left(\frac{\mu}{\nu}\, \rho\, a^2\, \mathrm{grad}\, \rho\right), \quad \text{where } \; a^2 = a^2(\rho) = \frac{dp}{d\rho} > 0. \tag{2.21}$$

We will investigate some of the consequences of a nonlinear diffusion coefficient in the problems *Nonlinear diffusion from a point source #nn* and *Nonlinear diffusion from a point seed* of the problem series: *Point Sources and Green's functions.*

3 Boundary integral methods.

Generally, Green's functions in analytic form can be obtained only for simple set-ups; e.g.: open space, half-spaces, and the like (for the diffusion or Laplace's equation). Furthermore, even in cases where an analytic form is "known", this form may be complicated; e.g: given by an infinite series, as in the case of rectangles for the heat equation in 2-D. The only situations where the Green's functions are "simple" are those where they follow by exploiting some symmetry in the problem (e.g.: full space), or where the method of images involves a small number of images only (e.g.: half space). Fortunately, it is some times possible to use "simple" Green's functions to reduce problems in "general" domains to lower-dimensional integral equations (which then must be solved numerically). This is the "main" idea behind the *Boundary Integral Methods (BIM)*, which we illustrate with simple examples in what follows.[15]

3.1 Toy example: heat equation in an interval.

Here we present an extremely simple BIM. The purpose of this section is illustrative only — as far as I know, the BIM here has no practical use.

Consider the problem

$$u_t = u_{xx} \quad \text{for } \; 0 < x < 1 \quad \text{and } \; 0 < t, \tag{3.1}$$

with boundary conditions $\boldsymbol{u(0,t) = a(t)}$ and $\boldsymbol{u(1,t) = b(t)}$, and initial condition $\boldsymbol{u(x,\,0) = f(x)}$, where a, b, and f are some given functions. *We will now show how to reduce this problem to that of finding two functions of a single variable, $\rho_0 = \rho_0(t)$ and $\rho_1 = \rho_1(t)$, defined on the boundary for the problem* — i.e.: $x = 0$ and $x = 1$.

Let $G = G(x,\,t)$ be the Green's function for the heat equation initial value in the whole line

$$G = \frac{1}{\sqrt{4\,\pi\,t}}\,\exp\left(-\frac{x^2}{4\,t}\right). \tag{3.2}$$

Similarly, let $H = H(x,\,t)$ be the Green's function for the half-line heat equation Dirichlet signaling problem. That is, H satisfies[16]

$$H_t = H_{xx} \quad \text{for } \; 0 < x \quad \text{and } \; -\infty < t < \infty, \tag{3.3}$$

with $\boldsymbol{H(0,\,t) = \delta(t)}$ and $\boldsymbol{H = 0}$ for $\boldsymbol{t < 0}$ (causality). Note that $H(-x,\,t)$ *satisfies the signaling problem for $x < 0$.* Now write[17]

$$u = \int_0^1 G(x-y,\,t)\,f(y)\,dy + \int_0^t H(x,\,t-s)\,\rho_0(s)\,ds + \int_0^t H(1-x,\,t-s)\,\rho_1(s)\,ds, \tag{3.4}$$

where the ρ_j are functions to be found. By construction this u satisfies the heat equation, and the initial condition $u(x,\,0) = f(x)$. Evaluating the expression at $x = 0$ and $x = 1$, and enforcing the boundary conditions, then yields

$$a(t) - \int_0^1 G(y,\,t)\,f(y)\,dy \;=\; \rho_0(t) + \int_0^t H(1,\,t-s)\,\rho_1(s)\,ds, \tag{3.5}$$

$$b(t) - \int_0^1 G(1-y,\,t)\,f(y)\,dy \;=\; \rho_1(t) + \int_0^t H(1,\,t-s)\,\rho_0(s)\,ds. \tag{3.6}$$

[15] A full development of the BIM theory is beyond the scope of this course.
[16] Finding H is the subject of the problem "Green's functions #05" in the series "Point Sources and Green's functions".
[17] Note that the integrals involving H_1 go only up to t because of causality.

This is a pair of **Volterra integral equations,** since they have the form

$$\rho_0(t) + \int_0^t \phi(t-s)\,\rho_1(s)\,ds = \text{known}, \tag{3.7}$$

$$\int_0^t \phi(t-s)\,\rho_0(s)\,ds + \rho_1(t) = \text{known}, \tag{3.8}$$

where $\phi(t) = H(1,\, t)$. Volterra equations have some very nice theoretical,[18] as well as numerical properties — for example, when discretized they yield either upper (or lower) diagonal systems, with ones in the diagonal, which can be solved by backward substitution.

Exercise 1:* *toy example with mixed boundary conditions. Write a BIM formulation for the problem where the left boundary condition in (3.1) is replaced by $\boldsymbol{u_x(0,\, t) = a(t)}$.

The End.

[18] For example: their solution by iteration generates a series that is rapidly convergent.