Lecture 4: Intermediate Asymptotics of Diffusion

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This lecture illustrates how idea of self-similarity can be used to solve partial differential equations, in the particular case of the diffusion equation. The method of "similarity" solutions generally works for the case where there is no natural choice of length scale available. In this lecture, two kinds of free-space diffusion problems are considered

1. diffusion from an arbitrary (localized) initial condition, and
2. a discrete random walk.

In each case, the leading order behavior is given by the self-similar Gaussian solution from before (= the Green function for the diffusion equation), but the higher order corrections are different in the two cases. In the former, corrections arise due to the structure of the initial concentration distribution, $C(x,0)$, and in the latter due to the discrete nature of the walk.

1 Diffusion from an arbitrary localized initial condition

Consider the diffusion equation and its initial and boundary conditions. For generality, assume that there are characteristic length scales, l_j in initial concentration profile $C_0(\vec{r})$. Also, consider infinite space domain where there is no mass source or sink, and thus total mass is conserved. This can be summarized in the following set of equations :

$$\frac{\partial C}{\partial t} = \mathcal{D}\nabla^2 C, \quad C(\vec{r},0) = C_0(\vec{r}), \quad C(\infty,t) = 0$$

<u>Invariant (Conservation of mass)</u> :

$$\int C(\vec{r},t)d\vec{r} = M_0 = \int C(\vec{r},0)d\vec{r}$$

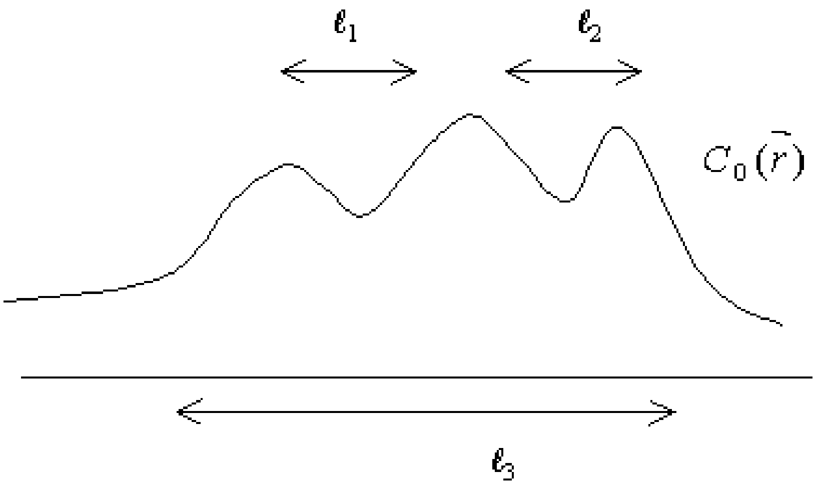

Figure 1: Various length scales

1.1 Dimensional Analysis

Variables in this system are

$$x, t, D, l_1, \cdots, l_j, M_0, C$$

There are $j+2$ dimensionless group in this system. The first $j+1$ dimensionless groups are from nondimensionalization of diffusion equation and initial condition as follows :

$$\zeta = \frac{x}{\sqrt{2Dt}}, \quad \eta_j = \frac{l_j}{\sqrt{2Dt}},$$

Note that characteristic scale for concentration cannot be obtained from normalizing diffusion equation or initial condition. This can be obtained from the invariant of system, mass conservation equation. If we choose the scale of concentration as follows,

$$[C] = M_0/(2Dt)^{d/2}$$

,or equivalently set up dimensionless concentration in the following form,

$$\tilde{C} = \frac{C(\vec{r}, t)}{M_0/(2Dt)^{d/2}}$$

one can show that the nondimensional form of mass conservation is turned into the following form :

$$\int \tilde{C} d\zeta = 1$$

Since only ζ, η_i and $\tilde{C}$ are dimensionless group in this system, the dimensionless concentration, $\tilde{C}$ can be expressed in the following form :

$$\boxed{\tilde{C} = \Phi(\zeta, \eta_j)}$$

In dimensional form:

$$\boxed{C(x,t) = \frac{M_0}{(2Dt)^{d/2}} \Phi\Big(\frac{r}{\sqrt{2Dt}}, \frac{l_j}{\sqrt{2Dt}}\Big)}$$

This in strict sense, though, is merely a conjecture, because it could fail to describe the system depending on the boundary condition.

Note that as $t \to \infty$ with fixed ζ, only M_0 is remembered and initial condition is forgotten, or $\eta_j = \frac{l_j}{\sqrt{2Dt}}$ term perishes due to diffusive mixing. Thus, in long time limit, Taylor expansion of Φ is possible with respect to η_j, if Φ is regular at $\eta_j = 0$. The expansion is given as follows :

$$\tilde{C} \sim \Phi(\zeta, 0) + \eta_j \frac{\partial \Phi}{\partial \eta_j}(\zeta, 0) + \cdots$$

It is worthwhile to mention that ζ is fixed, not x. If one lets $t \to \infty$ with x fixed, then $C \to 0$, which is too trivial. This is the reason it is called "intermediate limit" or "intermediate asymptotics".

1.2 Leading order intermediate asymptotics in d-dimensions

For now, neglect $\frac{l_j}{\sqrt{2Dt}}$ term and obtain leading term of diffusion equation, $\Phi(\zeta, 0)$ of the above expansion of $\tilde{C}$. The remaining higher order term will be obtained by perturbation theory, which will be mentioned later. The diffusion equation without initial conditions is as follows :

$$\frac{\partial C}{\partial t} = D\nabla^2 C, \quad M_0 = \text{initial mass}, \quad C(\infty, t) = 0$$

Above equation can be reformulated with new dimensionless variable ζ. LHS are using chain rule,

$$\begin{aligned}\frac{\partial C}{\partial t} &= \frac{M_0}{(2Dt)^{d/2}}\Big[-\frac{d}{2t}\Phi + \Phi'(\zeta)\frac{\zeta}{-2t}\Big] \\ &= -\frac{M_0}{(2t)^{d/2+1}D^{d/2}}[d\Phi + \zeta\Phi']\end{aligned}$$

RHS requires Laplacian operator in d-dimension. Though general Laplacian operator in d-dimension includes derivatives with respect to angle, the angular dependency can be neglected for long time limit due to diffusive mixing.

$$\begin{aligned}D\nabla^2 C &= D\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\Big(r^{d-1}\frac{\partial}{\partial r}\Big)C + \quad \text{(angular derivatives)} \\ &= D\Big(\frac{d-1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}\Big)C \\ &= \frac{DM_0}{(2Dt)^{d/2}}\Big(\frac{d-1}{r}\frac{\Phi'}{\sqrt{2Dt}} + \frac{\Phi''}{2Dt}\Big) \\ &= \frac{DM_0}{(2Dt)^{d/2+1}}\Big(\frac{d-1}{\zeta}\Phi' + \Phi''\Big)\end{aligned}$$

Therefore, equating LHS and RHS gives new ODE,

$$-(d\Phi + \zeta\Phi') = \frac{d-1}{\zeta}\Phi' + \Phi''$$

$$\boxed{\Phi'' + \Big(\zeta + \frac{d-1}{\zeta}\Big)\Phi' + d\Phi = 0}$$

The original partial differential equation of Φ with respect to x and t is transformed into an ordinary differential equation that depends solely on ζ. The similarity ansatz worked.

Now, we can solve this ODE subject to
boundary conditions:

$$\Phi(\infty) = 0$$

$$\Phi'(0) = 0 \quad : \text{(symmetry condition)}$$

normalization condition:

$$\int \Phi d\zeta = 1$$

The solution is as follows:

$$\boxed{\Phi(\zeta) = \frac{e^{-\zeta^2/2}}{(2\pi)^{d/2}}}$$

Putting dimensions back,

$$\boxed{C(\vec{r}, t) \sim \frac{M_0}{(4\pi Dt)^{d/2}} e^{-r^2/4Dt}}$$

NOTE :

- In the limit $t \to 0$, we have $C(\vec{r}, t) \to \delta(\vec{r}) M_0$.
- The leading order solution for $C(\vec{r}, t)$ in the intermediate (long-time) limit is equal to the exact solution in lecture 3 for the Green function $G(\vec{r}, t)$, except that the total mass is M_0 (rather than 1, in the case of the Green function).
- We never used initial condition, except in enforcing conservation of total mass.

In other words, any initial condition with the same total mass M_0 should lead to the same long time behavior, as if all the mass (random walkers) were originally concentrated at the origin at $t = 0$. All higher moments of the initial concentration distribution $C(\vec{r}, 0)$ beyond the zeroth (i.e. the total mass) are forgotten at leading order in the intermediate limit. However, the following example illustrates how higher moments play a role in the corrections to Gaussian leading order behavior.

1.3 Higher order corrections due to initial conditions

This example was not covered in the class. It is modified from handout of 2/15/01, Nigel Goldenfeld, "Lectures on Phase Transitions and the Renormalization Group" (Addison-Wesley, 1992)

Consider one dimensional diffusion equation :

$$\frac{\partial C}{\partial t} = \mathcal{D}\nabla^2 C, \quad -\infty < x < \infty$$

with initial condition in the form of Gaussian distribution.

$$C(x, 0) \sim \frac{M_0}{\sqrt{2\pi l^2}} e^{-x^2/2l^2}$$

By inspection, since the initial condition is of the same form as the similarity solution, the exact solution of this problem is,

$$C(x,t) \sim \frac{M_0}{\sqrt{2\pi(2Dt+l^2)}} e^{-x^2/2(2Dt+l^2)}$$

where essentially time has been shifted. In fact, if the solution is extended to negative time, we recover the usual initial condition for the Green function of the diffusion equation. Or, when $t = -l^2/2D$, one can show that

$$C\left(x, -\frac{l^2}{2D}\right) = M_0 \delta\left(t + \frac{l^2}{2D}\right)$$

Also, In long time limit with ζ =constant, or $t \gg l^2/2D$, we get the same leading order asymptotic approximation as before:

$$C(x,t) \sim \frac{M_0}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}$$

This is the same form of zeroth order intermediate asymptotics.

Since the exact answer is known, one can see the form of correction terms by obtaining Taylor expansion of exact solution. Define

$$\eta \equiv \frac{l}{\sqrt{2Dt}}, \quad \zeta \equiv \frac{x}{\sqrt{2Dt}}$$

Then,

$$\begin{aligned} C(\zeta;\eta) &= \frac{M_0}{\sqrt{4\pi Dt}} e^{-\frac{1}{2}\frac{\zeta^2}{1+\eta^2}} \frac{1}{\sqrt{1+\eta^2}} \\ &= \frac{M_0}{\sqrt{4\pi Dt}} e^{-\frac{\zeta^2}{2}} \left(1 + \left(\frac{1}{2}\zeta^2 - \frac{1}{2}\right)\eta^2 + \left(-\frac{3}{4}\zeta^2 + \frac{1}{8}\zeta^4 + \frac{3}{8}\right)\eta^4 + O\left(\xi^6\right)\right) \end{aligned}$$

It is clear that leading term is the same as what we've got in the zeroth order asymptotics and the correction terms are in the form of infinite series. Note that the first corrections are of order $\eta^2 = l^2/(2Dt)$. ♠

2 Intermediate Asymptotics of Random Walks

Consider the long time asymptotics of a walk with iid random steps :

$$C(\vec{r}, t+\tau) = \int p_\tau(\vec{r} - \vec{r}')C(\vec{r}', t)d\vec{r}'$$

Or, with Kramer-Moyal Expansion and D_n's,

$$\frac{\partial C}{\partial t}+\frac{\tau}{2}\frac{\partial^2 C}{\partial t^2}+\frac{\tau^2}{3!}\frac{\partial^3 C}{\partial t^3}+\cdots = D_2\frac{\partial^2 C}{\partial x^2}-D_3\frac{\partial^3 C}{\partial x^3}+D_4\frac{\partial^4 C}{\partial x^4}-\cdots$$

The leading term of Taylor expansion is obtained, one can look for correction terms. One should be cautious that previous section deals with correction of the initial condition, but this section is correction to the discreteness of transition probability. However, the zeroth order solution from previous section can be directly used here. The higher order term can be obtained essentially by including higher moments of transition probability. For the discrete iid random walk,

$$\frac{\partial C}{\partial t}\quad\underbrace{+\frac{\tau}{2}\frac{\partial^2 C}{\partial t^2}+\frac{\tau^2}{3!}\frac{\partial^3 C}{\partial t^3}+\cdots}_{\text{correction due to discrete time}}\quad = D_2\frac{\partial^2 C}{\partial x^2}\quad\underbrace{-D_3\frac{\partial^3 C}{\partial x^3}+D_4\frac{\partial^4 C}{\partial x^4}-\cdots}_{\text{corrections due to discreteness in space}}$$

Note that above equation does not have D_1. This is because we can always translate frame of reference with mean velocity or drift. Higher moments are, remembering from Fokker-Plank equation,

$$D_N = \frac{M_n}{n!\tau} = O(\tau^{n/2-1})$$

Since we have seen from our first lecture that $\delta x \sim \sqrt{\tau}$,

$$D_3 = O(\tau^{1/2})$$
$$D_4 = O(\tau)$$

Define $\mathcal{D}_n = D_n/\tau^{n/2-1}, n \geq 2$, then $\mathcal{D}_n \sim O(1)$. Combining these informations and reorganizing above equation give

$$\frac{\partial C}{\partial t}-\mathcal{D}_2\frac{\partial^2 C}{\partial x^2} = -\mathcal{D}_3\frac{\partial^3 C}{\partial x^3}\tau^{1/2}+\Big(\mathcal{D}_4\frac{\partial^4 C}{\partial x^4}-\frac{1}{2}\frac{\partial^2 C}{\partial t^2}\Big)\tau+O(\tau^{3/2})$$

$\cdot\mathcal{D}_3 \neq 0 \rightarrow$ homework "1b"
$\cdot\mathcal{D}_3 = 0, D_4 \neq 0$, symmetric walk.

$$\frac{\partial C}{\partial t}-\mathcal{D}_2\frac{\partial^2 C}{\partial x^2} = \Big(\mathcal{D}_4\frac{\partial^4 C}{\partial x^4}-\frac{1}{2}\frac{\partial^2 C}{\partial t^2}\Big)\tau+O(\tau^2)$$

where, $C = C_0+\tau C_1+\tau^2 C_2+\cdots$

We can solve this with symmetry transformation. With new dimensionless group, $\frac{\tau}{t} = \xi$ (effect of discreteness) [others : $\frac{\mathcal{D}_4}{2\mathcal{D}_2^2}$],

$$C(x,t) = \frac{M_0}{\sqrt{2\mathcal{D}_2 t}}\Phi\Big(\frac{x}{\sqrt{2\mathcal{D}_2 t}},\frac{\tau}{t}\Big)$$

,where $t \to \infty$, ζ fixed, ξ = small variable.

The order of magnitude of each term is as follows :

$$\underbrace{\frac{\partial C}{\partial t} - \mathcal{D}_2 \frac{\partial^2 C}{\partial x^2}}_{O(1)=O(\xi^0)} = \underbrace{\left(\mathcal{D}_4 \frac{\partial^4 C}{\partial x^4} - \frac{1}{2}\frac{\partial^2 C}{\partial t^2}\right)\tau}_{O(\xi^1)} + \underbrace{O(\tau^2)}_{O(\xi^2)}$$

We can use perturbation expansion.

$$\tilde{C} = \tilde{C}_0 + \xi \tilde{C}_1 + \xi^2 \tilde{C}_2 + \cdots$$

$$\tilde{C}(\zeta, \xi) = \underbrace{\tilde{C}_0(\zeta, 0)}_{\Phi(\zeta,0)} + \xi \underbrace{\tilde{C}_1(\zeta, 0)}_{\frac{\partial \Phi}{\partial \xi}(\zeta,0)} + \xi^2 \underbrace{\tilde{C}_2(\zeta, 0)}_{\frac{1}{2}\frac{\partial^2 \Phi}{\partial \xi^2}(\zeta,0)} + \cdots$$

Note that $\tilde{C}$ is the same as the long time solution from section 1. We will solve this in next class.