§6 Boundary conditions for the Fokker-Planck equation

- We need to consider the different types of boundary conditions for the FPE, with a view towards applications. We’ll mostly use the 1D case for examples, but all boundary conditions have higher-dimensional analogues also.

1. Natural boundary conditions

- This is the condition we have used in most of our examples so far: $P(x, t) \to 0$ as $x \to \infty$ or $x \to -\infty$, with the decay to zero being sufficiently fast to ensure the normalization integral is

$$\int_{-\infty}^{\infty} P(x, t) \, dx = 1.$$ 

In the 1D case this requires $P(x, t) \to 0$ faster than $|x|^{-1}$ as $|x| \to \infty$.

- The natural BC typically is applied when the range of the random variable $x(t)$ is infinite or semi-infinite.

- We saw an example of natural BCs in two dimensions also: for the nonlinear oscillator example we had $P_\infty \to 0$ as $r \to \infty$.

2. Reflecting boundary conditions

- For e.g. Brownian particles near a wall, the wall provides an impenetrable barrier.

- We write the FPE for $P(x, t)$ in the form

$$\frac{\partial P}{\partial t} + \frac{\partial S}{\partial x} = 0,$$

where $S(x, t)$ is the “probability flux (or current)” [Risken p. 84] given for

$$\dot{x} = f(x) + g(x)\eta(t)$$

as

$$S(x, t) = f(x)P(x, t) - \kappa g(x) \frac{\partial}{\partial x} [g(x)P(x, t)].$$

- The name for $S$ can explained by considering the rate of change of probability (or concentration of Brownian particles) between two fixed positions $x = A$ and $x = B$:

$$\frac{d}{dt} \int_A^B P(x, t) \, dx = \int_A^B \frac{\partial P}{\partial t} \, dx = - \int_A^B \frac{\partial S}{\partial x} \, dx = S(A, t) - S(B, t).$$

- This is interpreted as:

rate of change of probability of being in $[A, B] = \text{(flow into } [A, B] \text{ through } x = A) - \text{(flow out of } [A, B] \text{ through } x = B)$. 

• Thus $S(x, t)$ represents the flow or flux of particles (or current) through the point $x$ at time $t$.

• Now suppose there is an impenetrable wall at some position $x = a$.

• Since particles cannot penetrate the wall the flux at $x = a$ must be zero:

$$\Rightarrow S(a, t) = 0$$

for all $t$.

• This provides the boundary condition at $x = a$:

$$f(a)P(a, t) - \kappa g(x) \frac{\partial}{\partial x} [g(x)P(x, t)] \bigg|_{x=a} = 0.$$ 

• This simplifies in many common cases.

• E.g. Brownian motion with $f \equiv 0$ and $g \equiv 1$. We have seen the use of natural boundaries when the particles can move freely in the infinite interval $x \in (-\infty, \infty)$. Suppose there is an impenetrable wall at $x = a$, so the particles are constrained to move in the semi-infinite interval $x \in (-\infty, a]$.

• The FPE is

$$\frac{\partial P}{\partial t} = \kappa \frac{\partial^2 P}{\partial x^2}$$

with initial condition $P(x, 0) = \delta(x)$ as before.

• The boundary conditions are:

$$P(x, t) \to 0 \text{ as } x \to -\infty$$

(natural BC) and a no-flux BC at $x = a$:

$$\kappa \frac{\partial P}{\partial x} \bigg|_{x=a} = 0,$$

or simply

$$\frac{\partial P}{\partial x} \bigg|_{x=a} = 0.$$

• The probability flux can be defined for higher-dimensional problems also [Risken p.84], e.g. for the convection-diffusion problem

$$\dot{x} = v(x) + \eta(t)$$
with
\[ \langle \eta_i(t)\eta_j(t') \rangle = 2\kappa \delta_{ij} \delta(t-t'), \]
we found the FPE
\[ \frac{\partial P}{\partial t} = -\nabla \cdot (vP) + \kappa \nabla^2 P. \]

- The FPE may be written in terms of the probability flux vector \( S \) as
\[ \frac{\partial P}{\partial t} + \nabla S = 0 \]
and
\[ S(x, t) = v(x)P(x, t) - \kappa \nabla P(x, t). \]

- Consider a 2D example, with a wall at \( y = a \).

- Writing \( \hat{n} \) as the (outward) unit normal vector at the wall, the no-flux condition is
\[ \hat{n} \cdot S = 0 \]
\[ \Rightarrow [v \cdot \hat{n} P - \kappa \hat{n} \cdot \nabla P]_{y=a} = 0. \]

- For fluid flows, the velocity vector \( v(x) \) has no component perpendicular to the wall, so \( v \cdot \hat{n} = 0 \) at \( y = a \).

- Thus the no-flux BC is
\[ \hat{n} \cdot \nabla P = 0 \]
at the wall; in other words the normal derivative of \( P \) is zero at the wall. In our example with the wall at \( y = a \), this yields
\[ \frac{\partial P}{\partial y} \bigg|_{y=a} = 0. \]

3. Absorbing boundary conditions

- An absorbing wall at \( x = a \) means that particles are removed from the interval \((-\infty, a]\) as soon as they first hit \( x = a \).

- This can occur for physical reasons (e.g. a chemical reaction at the wall causes molecules to be absorbed or changed to a different chemical species), or for mathematical reasons (we will impose absorbing BCs when looking at first passage time problems).

- The appropriate BC for an absorbing wall at \( x = a \) is
\[ P(a, t) = 0, \]
i.e. zero probability of finding particles at the wall, since they are immediately absorbed.
**Example:** A microelectrode recessed into a surface. Concentration of ions in bulk is $c_b$. Consider the electrode to be at $z = 0$, with the flat surface at $z = L$.

- The Langevin equation for the freely diffusing ions (take 1D approx for a long, narrow recess) with vertical position $z(t)$ is
  \[
  \frac{dz}{dt} = \eta(t)
  \]
  with $\langle \eta(t)\eta(t') \rangle = 2\kappa\delta(t - t')$.

- The FPE for the PDF $P(z, t)$ (or concentration $c(z, t) \equiv P(z, t)$) is
  \[
  \frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial z^2},
  \]
  with absorbing BC at $z = 0$:
  \[
  c(0, t) = 0.
  \]

- The other boundary condition is
  \[
  c(L, t) = c_b,
  \]
  assuming the concentration at the mouth of the recess is equal to the bulk concentration.

- Our goal is to find the steady-state current at the electrode in terms of $c_b$ and $L$.

- The electrode current is proportional to the probability flux at $z = 0$, i.e.,
  \[
  I = \beta \frac{\partial c}{\partial z} \Big|_{z=0}
  \]
  for appropriate constant $\beta$ (since current is proportional to rate of change of charge = flux of ions onto electrode).

- In steady state, $c = c_\infty(z)$ and
  \[
  \frac{d^2 c_\infty}{dz^2} = 0.
  \]

- Solution:
  \[
  c_\infty(z) = Az + B
  \]
  for constants $A$ and $B$.

- Applying boundary conditions gives $B = 0$ and $A = \frac{c_b}{L}$, so
  \[
  c_\infty(z) = \frac{c_b z}{L}.
  \]

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• Then

\[ \frac{dc_\infty}{dz} = \frac{c_b}{L} \]

and so

\[ I = \beta \frac{c_b}{L} \]

gives the electrode current dependence on \( c_b \) and \( L \).

• 4. Periodic boundary conditions

• If the random variable is naturally periodic, e.g., an angular variable with \( \theta \in [0, 2\pi] \) then periodic boundary conditions must be imposed on the FPE [Risken p.103]:

\[
P(\theta + 2\pi, t) = P(\theta, t) \\
S(\theta + 2\pi, t) = S(\theta, t)
\]

• Example: the phase angle for a nonlinear oscillator, with strong amplitude control (so \( r \equiv 1 \)).

• Motion is restricted to the limit cycle, with deterministic rotation frequency \( \Omega \), plus noise effects:

\[ \dot{\theta} = \Omega + \text{noise terms} \]

• Then PDF \( P(\theta, t) \) is defined only for \( \theta \in [0, 2\pi] \) with

\[ P(0, t) = P(2\pi, t) \]

and

\[ S(0, t) = S(2\pi, t). \]