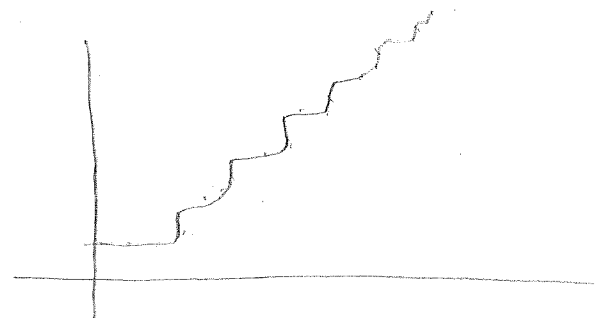
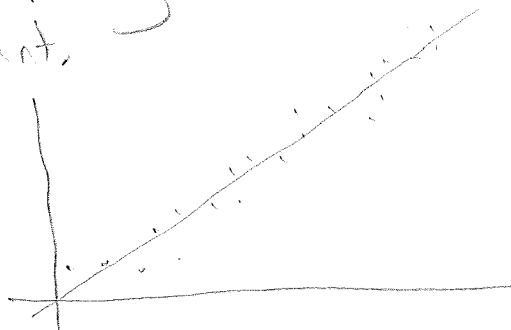


So far, we have only looked at deterministic processes - that is, processes where knowing the state right now tells you everything that will happen in the future. Even extremely complicated chaotic dynamics like those of $x_{t+1} = 3.9x_t(1-x_t)$ are still deterministic. In the real world, though, things are seldom so regimented. There are several pervasive sources of randomness in the world.

- Quantum Mechanics: At a fundamental level, particles do not behave in a deterministic manner. This is the hardest to argue with, but probably the least important for modelling. Large objects are not strongly influenced by quantum effects.

- Measurement Error: Even if the world really were perfectly deterministic, we would still make mistakes while measuring it. A good model should take this into account.



(P.5)
1) The chance of not decaying now is independent of the chance of not decaying in the past. That is,
$$P(t + \Delta t) = P(t) \cdot P(\Delta t).$$

2) Over very small time intervals, the chance of decaying is approximately linear. That is,

$$1 - P(\Delta t) = \lambda \Delta t + \underbrace{o(\Delta t)}$$

$\hookrightarrow o(\Delta t)$ means

$$\lim_{\Delta t \rightarrow 0} \frac{o(\Delta t)}{\Delta t} = 0$$

We therefore have:

$$P(t + \Delta t) = P(t) \cdot P(\Delta t)$$

$$= P(t) \cdot [1 - \lambda \Delta t - o(\Delta t)]$$

$$\Rightarrow P(t + \Delta t) - P(t) = -\lambda \Delta t P(t) - o(\Delta t) P(t)$$

$$\Rightarrow \frac{P(t + \Delta t) - P(t)}{\Delta t} = -\lambda P(t) - \frac{o(\Delta t)}{\Delta t} P(t)$$

$$\Rightarrow \frac{dP}{dt} = -\lambda P(t)$$

$$\Rightarrow P(t) = A e^{-\lambda t}$$

• Aggregate Effects: The impacts of many P.2
small (maybe deterministic) events can
appear random in aggregate. If we do not
understand these events, or cannot model them
well, it is usually better to treat them
as random. This may seem like the flimsiest
argument, but it turns out to be the most
important in most modeling.

Example: A hot topic in biomechanics is understanding
how proteins fold. A protein is a chain
of small(ish) molecules called amino acids. When
in water, the protein spends most of its time
folded into a few specific shapes. People want
to know what those shapes are and how the protein
gets there. To understand this shape, you want
to know the dynamics of all the atoms in the
protein, which are strongly affected by the
dynamics of nearby water molecules.

This is already a big enough system that quantum
effects are probably washed out, but measurement
error is still a factor. We can only get
approximate locations of atoms in the protein.

and we have no idea where the H_2O is. (P.3)

More importantly, modeling all the water molecules is very hard. We know (essentially) the rules for how atoms interact, so we can choose arbitrary starting positions for H_2O , then numerically solve a big system of differential equations and find out where all the atoms go.

Unfortunately, there are (on the low end) hundreds of atoms in the protein and thousands in the water. State of the art (a few years ago) could model this system for 10 microseconds, and that took weeks to solve.

This is just long enough to see the smallest proteins fold once, but often into an uninteresting configuration.

A much more feasible plan is to think of the water as applying random forces, and then only model the protein explicitly.

(P.4)

We will start with a much simpler example. Radioactive isotopes decay with a characteristic rate. You've probably seen the equation

$$N(t) = N_0 e^{-\lambda t}$$

used to describe this decay, what is N ? It's often described as the number of atoms, but that can't be right - $N(t)$ is not a whole number most of the time. It could also be the density of atoms in some fixed volume. That makes a little more sense, but the number of atoms is still discrete. In particular, what if there was only one atom? It either decays or it doesn't, so N is either 1 or 0; it doesn't drop exponentially.

The decay of a single atom really is random, so it makes sense to describe it in terms of probability. We will let $P(t)$ be the probability that our atom has not decayed by time t . We will make two assumptions about P .

Really, our notation has been a little sloppy. (P. 6)

We should say that the time of decay T is a random variable. The probability that our atom decays by time t is:

$$\text{Pr}[T \leq t] = 1 - P(t) = 1 - e^{-\lambda t}.$$

This is the cumulative distribution function (cdf) of T . We often are interested in the probability density function (pdf)

$$f_T(t) = \frac{d}{dt} \text{Pr}[T \leq t] = \lambda e^{-\lambda t}.$$

From the cdf/pdf, we can find any statistics we want about T . For instance, the mean of T is

$$\begin{aligned} \langle T \rangle &= \int_0^{\infty} t f_T(t) dt = \int_0^{\infty} t \lambda e^{-\lambda t} dt \\ &= t \cdot \left. -\frac{1}{\lambda} e^{-\lambda t} \right|_0^{\infty} + \int_0^{\infty} \frac{1}{\lambda} e^{-\lambda t} dt \\ &= \left. -\frac{1}{\lambda} e^{-\lambda t} \right|_0^{\infty} = \frac{1}{\lambda}. \end{aligned}$$

That is, the average time to decay is $1/\lambda$ the rate of decay.

$$\text{Var}(T) = \langle T^2 \rangle - \langle T \rangle^2 = \int_0^{\infty} t^2 \lambda e^{-\lambda t} dt - \frac{1}{\lambda^2}$$

What's the expected number of atoms at time t ?

$$\langle N(t) \rangle = 0 \cdot \text{Pr}[N(t)=0] + 1 \cdot \text{Pr}[N(t)=1]$$

$$= 0 \cdot \text{Pr}[T \leq t] + 1 \cdot \text{Pr}[T > t]$$

$$= 0 + e^{-\lambda t}$$

$$= e^{-\lambda t}$$

What if we have two atoms sitting next to each other? We will assume they don't affect each other (they are i.i.d.). (P.2)

(A)

(B)

Let T_A be the time that atom A decays and T_B be the time that atom B decays

We know that $\Pr[T_A \leq t] = \Pr[T_B \leq t] = 1 - e^{-\lambda t}$.

What is the probability that neither has decayed at time t ? That is, that $T_A > t$ and $T_B > t$.

Since T_A and T_B are independent,

$$\begin{aligned}\Pr[T_A > t \text{ and } T_B > t] &= \Pr[T_A > t] \cdot \Pr[T_B > t] \\ &= e^{-\lambda t} \cdot e^{-\lambda t} = e^{-2\lambda t}.\end{aligned}$$

Likewise, the probability that both decayed by time t is

$$\begin{aligned}\Pr[T_A \leq t \text{ and } T_B \leq t] &= \Pr[T_A \leq t] \cdot \Pr[T_B \leq t] \\ &= (1 - e^{-\lambda t}) \cdot (1 - e^{-\lambda t}) = 1 - 2e^{-\lambda t} + e^{-2\lambda t}.\end{aligned}$$

Finally, what's the probability that one decayed and one did not? P.8

$$\begin{aligned} & \Pr[(T_A \leq t \text{ and } T_B > t) \text{ or } (T_A > t \text{ and } T_B \leq t)] \\ &= (1 - e^{-\lambda t}) \cdot e^{-\lambda t} + e^{-\lambda t} \cdot (1 - e^{-\lambda t}) \\ &= 2[e^{-\lambda t} - e^{-2\lambda t}] = 2e^{-\lambda t} - 2e^{-2\lambda t} \end{aligned}$$

What's the expected number of atoms remaining?

$$\begin{aligned} \langle N(t) \rangle &= 0 \cdot \Pr[N(t)=0] + 1 \cdot \Pr[N(t)=1] + 2 \cdot \Pr[N(t)=2] \\ &= 0 \cdot \Pr[\text{both decayed}] + 1 \cdot \Pr[\text{one decayed}] + 2 \cdot \Pr[\text{no decays}] \\ &= 1 \cdot (2e^{-\lambda t} - 2e^{-2\lambda t}) + 2 \cdot e^{-2\lambda t} \\ &= 2e^{-\lambda t} \end{aligned}$$