Misc

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1 Exponential distribution

Suppose the probability of something happening in an interval Δt equals $a_0\Delta t$. This means that the probability it happens

- in the first interval is just $a_0\Delta t$,
- in the second interval is $(1 - a_0\Delta t) \times a_0\Delta t$ (i.e. the probability it doesn't happen in the first interval multiplied by the probability that it does happen in the second)
- ...
- in the n^{th} interval is $(1 - a_0\Delta t)^{n-1} \times a_0\Delta t$

Now suppose we call $T = n\Delta t$, then the probability that the event happens in the interval $[T, T + \Delta t]$, is just the same:

$$\mathrm{prob}(T, T + \Delta t) = (1 - a_0\Delta t)^{n-1} \times a_0\Delta t$$

If we look at this in terms of some probability density, we can write:

$$\mathrm{prob}(T, T + \Delta t) = \int_T^{T+\Delta t} \mathrm{prob}(s)\mathrm{d}s \approx \mathrm{prob}(T)\Delta t,$$

assuming very small intervals. We can then rewrite the previous equation as

$$\mathrm{prob}(T) = (1 - a_0\Delta t)^{n-1} \times a_0 = a_0(1 - a_0\Delta t)^{\frac{T-\Delta t}{\Delta t}},$$

which for infinitely small intervals becomes an exponential:

$$\mathrm{prob}(T) = a_0 \exp(-a_0 T)$$

So if the probability of some event happening in an infinitesimal interval $\mathrm{d}t$ is $a_0\mathrm{d}t$, then the probability density for the event happening at time T is given by the formula above, an exponential distribution.

2 Poisson distribution

Suppose we start from some exponential distribution with parameter λ

$$\text{prob}(x_1|\lambda) = \lambda \exp(-\lambda x_1)$$

, giving us the probability density for obtaining a number x_1 from this distribution (if x_1 is positive, the probability for a negative number is zero). If the probability density for obtaining another number x_2 is the same,

$$\text{prob}(x_2|\lambda) = \lambda \exp(-\lambda x_2)$$

, we could wonder wat the probability density is for $y_2 = x_1 + x_2$, the sum of two such numbers. Of course, since x_1 and x_2 are independent, the joint probability density is just

$$\text{prob}(x_1, x_2|\lambda) = \lambda^2 \exp(-\lambda x_1 - \lambda x_2)$$

if both x_1 and x_2 are positive.

By introducing another variable $y_2' = x_1 - x_2$, we can transform the joint probability density for x_1 and x_2 into one for y_2 and y_2':

$$\text{prob}(y_2, y_2') = \text{prob}\left(x_1(y_2, y_2')\right) \text{prob}\left(x_2(y_2, y_2')\right) \times \frac{1}{2},$$

where the factor $\frac{1}{2}$ comes from the Jacobian determinant of the transformation between variables. The condition that both x_1 and x_2 must be positive, becomes:

$$-y_2 < y_2' < y_2,$$

otherwise the joint probability density is zero. Some algebra yields

$$\text{prob}(y_2, y_2') = \frac{\lambda^2}{2} \exp(-\lambda y_2)$$

To get the probability density for the y_2, i.e. the sum of x_1 and x_2, we just have to marginalize y_2':

$$\text{prob}(y_2) = \int_{-y_2}^{y_2} \mathrm{d}y_2' \frac{\lambda^2}{2} \exp(-\lambda y_2) = \lambda^2 y_2 \exp(-\lambda y_2),$$

where the integration interval comes from the fact that the density is zero otherwise.

This can be repeated for the sum of more events, and if we call s_i the sum of i events with the same exponential distribution, we find

$$\begin{aligned}
\text{prob}(s_1) &= \lambda \exp(-\lambda s_1) \\
\text{prob}(s_2) &= \lambda^2 s_2 \exp(-\lambda s_2) \\
\text{prob}(s_3) &= \frac{\lambda^3}{2} s_3^2 \exp(-\lambda s_3) \\
\text{prob}(s_4) &= \frac{\lambda^4}{2 \times 3} s_4^3 \exp(-\lambda s_4) \\
&\cdots \\
\text{prob}(s_n) &= \frac{\lambda^n}{(n-1)!} s_n^{n-1} \exp(-\lambda s_n)
\end{aligned}$$

So for underlying numbers from an exponential distribution we can write:

$$\text{prob}(x|n\text{ events},\lambda) = \frac{\lambda^{\mathrm{n}}}{(\mathrm{n}-1)!}\mathrm{x}^{\mathrm{n}-1}\exp(-\lambda\mathrm{x}),$$

the probability density that the sum of n numbers equals x. Using Bayes' rule with a Jeffrey's prior for n and x, we get:

$$\text{prob}(n\text{ events}|\mathrm{x},\lambda) = \frac{1}{\mathrm{n}!}(\lambda\mathrm{x})^{\mathrm{n}}\exp(-\lambda\mathrm{x})$$

Calling the average of this probability μ, we get:

$$\mu = \sum_{n=0}^{\infty} n \times \text{prob}(n\text{ events}|\mathrm{x},\lambda) = \lambda\mathrm{x}$$

which finally yields the Poisson distribution:

$$\text{prob}(n\text{ events}|\mu) = \frac{\mu^{\mathrm{n}}\exp(-\mu)}{\mathrm{n}!}$$

3 Poisson process

Suppose we can pick times from an exponential distribution $\text{prob}(t) = \exp(-t)$, yielding a list of time intervals Δt_1, Δt_2, ... We shall interpret these intervals as the time between certain events, so the first event occurs at $t_1 = \Delta t_1$, the second at $t_2 = t_1 + \Delta t_2$, so Δt_2 later, etc. Generating event times in this way is called a *unit rate Poisson process*.

We can then define a function $Y(t)$, which returns the number of events that took place until time t. So this function is zero before t_1 and makes a jump to one at t_1. Then, at t_2 the function jumps to value two, and so on. Based on this function Y we can also define another function

$$Y_\lambda(t) \equiv Y(\lambda t)$$

, meaning that we'll be progressing faster or slower along the event time line. Note that this is the same as if we'd start from a probability distribution $\text{prob}(t) = \lambda\exp(-\lambda t)$.

Using Y_λ, we can look at the probability that a specific number of events happened in a certain time interval:

$$\text{prob}(Y_\lambda(t+\Delta t) - Y_\lambda(t) = n),$$

which just follows a Poisson distribution:

$$\text{prob}(Y_\lambda(t+\Delta t) - Y_\lambda(t) = n) = \frac{(\lambda t)^n\exp(-\lambda\Delta t)}{n!}$$

This means that the probability that at least one event happens is

$$\text{prob}(Y_\lambda(t+\Delta t) - Y_\lambda(t) > 0) = 1 - \text{prob}(Y_\lambda(t+\Delta t) + Y_\lambda(t) = 0) = 1 - \exp(-\lambda\Delta t),$$

which for a small interval can be approximated as

$$\text{prob}(Y_\lambda(t+\Delta t) - Y_\lambda(t) > 0) \approx \lambda\Delta t$$

Instead of a uniform speedup or slowdown, we can also use a more general mapping to a unit-rate Poisson process, using a 'propensity function' or 'hazard' $a(t)$:

$$Y_a(y) \equiv Y(T(t)),$$

where

$$T(t) = \int_0^t a(s)\mathrm{d}s$$

specifies the mapping between the real time t and the time for the unit-rate process T. The probability that an event fires in Δt after time t, then becomes

$$\mathrm{prob}(Y_a(t + \Delta t) - Y_a(t) > 0) \approx a(t)\Delta t,$$

again for a small interval.

4 Simulation state

We're going to use such a Poisson process to base an event based simulation on. For now, we'll be working with propensity functions that only depend on time through $X(t)$, the state of the simulation at time t. Furthermore, this simulation state will only change at times at which events fire.

Suppose we have two types of events, A and B, firing based on a non-uniform Poisson process. At some time t_0, for example the start of the simulation, two event fire times have been calculated, one for A (t_A) and one for B (t_B). These have both been calculated based on the state at time t_0, so based on $X(t_0)$.

The times t_A and t_B correspond to times of the unit-rate poisson process T_A and T_B and it is from this unit-rate Poisson process that the random times are picked. They are then mapped to actual event times using the mappings

$$T_A = \int_{t_0}^{t_A} a(X(t_0))\mathrm{d}s$$

$$T_B = \int_{t_0}^{t_B} b(X(t_0))\mathrm{d}s \tag{1}$$

where a and b are the propensity functions for the two processes. Note that in the integral it says $X(t_0)$, indicating that the calculations are based on the state of the simulation at time t_0. Also note that it's the T values that are generated from the unit rate Poisson process, and that the equations need to be solved for arguments in the integral boundaries.

When these t times are first calculated, it is unknown which one will fire first. For this argument, well assume that it's an event from process A that fires first, at t_A. While the T_B value is still correct (it is just generated from a unit rate Poisson process), the mapping to t_B is no longer correct if the firing of the A event has changed the state.

Remember that the state X can only change at event times, so in this case, the new mapping for the time of the B event, let's call it t_B^N should correspond to:

$$T_B = \int_{t_0}^{t_A} b(X(t_0))\mathrm{d}s + \int_{t_A}^{t_B^N} b(X(t_A))\mathrm{d}s \tag{2}$$

$$\Leftrightarrow T_B = \int_{t_0}^{t_B} b(X(t_0))\mathrm{d}s - \int_{t_A}^{t_B} b(X(t_0))\mathrm{d}s + \int_{t_A}^{t_B^N} b(X(t_A))\mathrm{d}s \tag{3}$$

Comparing (1) and (3), one sees that t_B^N should satisfy

$$\int_{t_A}^{t_B} b(X(t_0))\mathrm{d}s = \int_{t_A}^{t_B^N} b(X(t_A))\mathrm{d}s \tag{4}$$

In this particular scenario, we're assuming that the propensities only change at the times the events fire, so here $b(X(t_0)) = b_0 = \text{const}$ and $b(X(t_A)) = b_A = \text{const}$. The equation above then becomes

$$(t_B - t_A)b_0 = (t_B^N - t_A)b_A \tag{5}$$
$$\Leftrightarrow t_B^N = t_A + \frac{b_0}{b_A}(t_B - t_A)$$

Since t_B was already calculated and t_A is also known, we know the new real-world fire time for the event from process B when we have calculated the value $b_A = b(X(t_A))$ of the propensity for the new state of the system, i.e. after it has been modified by A at t_A.

Equation () also suggest that we can look at it another way. Because the propensity is a constant in between event firings, the product of a time interval and the propensity corresponds to a change in internal unit-rate process time T. The equation says that the internal interval we first expected from time t_A to t_B was $(t_B - t_A)b_0$, but due to the change in propensity this interval should now be mapped onto $(t_B^N - t_A)b_A$, yielding a new event time t_B^N.

Another way of looking at things is suggested by (2). It says that we can first calculate a new value T'_B,

$$T'_B = T_B - \int_{t_0}^{t_A} b(X(t_0))\mathrm{d}s \tag{6}$$

which adjusts the internal event time for the time that has passed until A fired at t_A. Then, the new event time t_B^N is calculated by equating this remaining internal time T'_B to the integral as usual:

$$T'_B = \int_{t_A}^{t_B^N} b(X(t_A))\mathrm{d}s$$

Using this integral form also works for more general time dependent propensities, which not only depend on the state (still only changing at event fire times), but also on a time parameter:

$$T(t) = \int_0^t a(X(s), s)\mathrm{d}s$$

5 Time-dependent modified Next Reaction Method

5.1 Core algorithm

Instead of calling internal times T, we'll call them ΔT to indicate that they're time intervals that will be modified by the procedure from (6). Suppose there are M possible reactions, and call $rnd()$ a function that returns a random number in $[0, 1]$ (uniform). The time-dependent modified Next Reaction Method then works as follows:

- Initialization:
  1. for k from 1 to M, $\Delta T_k = \log\left(\frac{1}{rnd()}\right)$
     This picks numbers from an exponential distribution $p(x) = \exp(-x)$ and correspond to the initial internal fire times for the different event types (which still need to be mapped onto real world times using the propensities).
  2. set $t = 0$
- Loop:

1. for k from 1 to M, calculate Δt_k so that $\Delta T_k = \int_t^{t+\Delta t_k} a_k(X(t), s)ds$
   This translates the time left from the exponential distribution (the Poisson process) into a physical time that should pass until the event fires.
2. call μ the index for which $\Delta t_\mu = \min(\Delta t_1, ..., \Delta t_M)$
   This is the event that shall fire first.
3. for k from 1 to M except μ, change ΔT_k to $\Delta T_k - \int_t^{t+\Delta t_\mu} a_k(X(t), s)ds$
   Note that because Δt_μ is the smallest of them all, the integral will be smaller than the one in 1, and ΔT_k will stay positive (unless there's some really strange propensity function, which of course should not happen)
4. add Δt_μ to t
5. fire event μ which can change the simulation state
6. set $\Delta T_\mu = \log\left(\frac{1}{rnd()}\right)$
   For this particular event, no next one had been calculated, so we need to pick a new internal time from an exponential distribution (again for the poisson process)

5.2 An optimization

It may not be necessary to do the $\int_t^{t+\Delta t_\mu} a_k(X(t), s)ds$ calculation every time. If the propensity function changes due to each event, then we really do need to calculate every

$$\Delta T_{k,1} = \int_{t_0}^{t_1} a_k(X(t), s)ds,\ \Delta T_{k,2} = \int_{t_1}^{t_2} a_k(X(t), s)ds,\ \Delta T_{k,3} = \int_{t_2}^{t_3} a_k(X(t), s)ds, \text{ etc.}$$

However, if the propensity does not change for a particular event k, then instead of calculating each $\Delta T_{k,i}$ above, we can save some unnecessary recalculations by just calculating an integral

$$\Delta T_{k,sum} = \int_{t_0}^{t_{end}} a_k(X(t), s)ds$$

when really needed.

To make this work, some additional bookkeeping is needed to be able to determine when the events would fire in real time.

- Initialization:
  1. for k from 1 to M, $\Delta T_k = \log\left(\frac{1}{rnd()}\right)$
     This picks numbers from an exponential distribution $p(x) = \exp(-x)$
  2. set $t = 0$
  3. for each k, we must also know the time at which this calculation of ΔT took place. For now this is just $t = 0$, so we set $t_k^c = 0$ for all k.
  4. for each k, map these internal Poisson intervals ΔT_k to event fire times t_k^f using the propensities:
     $$\Delta T_k = \int_{t_k^c}^{t_k^f} a_k(X(t_k^c), s)ds$$
- Loop:

1. for k from 1 to M, calculate the minimum real time that would elapse until an event: $\Delta t_\mu = \min(t_1^f - t, ..., t_M^f - t)$. Here μ is the index of the event that corresponds to this minimal value.
2. add Δt_μ to t
3. only for the events k for which the propensities will be affected by μ, we need to do the following:
   - Diminish the internal time ΔT_k with the internal time that has passed:

     $$\Delta T_k := \Delta T_k - \int_{t_k^c}^{t} a_k(X(t_k^c), s) ds$$

     Here t is the new time, and the propensities are still the *old* propensities!
   - Set $t_k^c = t$
4. fire event μ (change state vector), generate a new random number and ΔT value, set $t_\mu^c = t$ and calculate t_μ^f accordingly.
5. only for the events k for which the propensities were affected by μ, we need to recalculate the real fire times of these events: calculate t_k^f so that this holds:

   $$\Delta T_k = \int_{t_k^c}^{t_k^f} a_k(X(t_k^c), s) ds$$

   Note that here we're working with the *new* propensities.

If one keeps track of which event affects which, this can really save some calculation time. Furthermore, if certain events are stored in a list sorted on real event fire times, the minimum may very easily be calculated: if these times increase, one will only need to look at the first event instead of them all.

One might argue that keeping such a list ordered may require some computation as well, but if the list (or a part of it) does not need to be updated due to a certain event, no computation is needed for that part.

A slightly re-ordered version (for positive times only since we use a negative one as a marker):

- Initialization:
  1. set $t = 0$
  2. for k from 1 to M, let $\Delta T_k = \log\left(\frac{1}{rnd()}\right)$ (this picks numbers from an exponential distribution $p(x) = \exp(-x)$). Set $t_k^c = 0$ and set $t_k^f = -1$ to indicate that this event time still needs to be calculated from the ΔT_k version.
- Loop:
  1. for k from 1 to M, if $t_k^f < 0$ then calculate t_k^f from the stored ΔT_k value so that:

     $$\Delta T_k = \int_{t_k^c}^{t_k^f} a_k(X(t_k^c), s) ds$$

  2. for k from 1 to M, calculate the minimum real time that would elapse until an event takes place: $\Delta t_\mu = \min(t_1^f - t, ..., t_M^f - t)$. Here μ is the index of the event that corresponds to this minimal value.

3. add Δt_μ to t
4. only for the events k for which the propensities will be affected by μ, we need to do the following:
   - Diminish the internal time ΔT_k with the internal time that has passed:

     $$\Delta T_k := \Delta T_k - \int_{t_k^c}^{t} a_k(X(t_k^c), s) ds$$

     Here t is the new time, and the propensities are still the *old* propensities!
   - Set $t_k^c = t$ and set $t_k^f = -1$ to indicate that it still needs to be calculated from the remaining ΔT_k.
5. fire event μ (change state vector), generate a new random number and ΔT value, set $t_\mu^c = t$ and set $t_\mu^f = -1$ to indicate that t_c^f should be calculated from ΔT_μ.

6 Probability distribution for a propensity/hazard

For the mNRM method, we started from random numbers drawn from the exponential probability distribution $\mathrm{prob}(T) = \exp(-T)$, used as 'internal' times by the algorithm. These are mapped onto real-world times by using a certain propensity function or hazard, providing a relation between real-world time and internal time

$$T(t) = \int_0^t h(s) \mathrm{d}s,$$

where $h(t)$ is the hazard.

This means that in terms of t, the probability density becomes

$$\mathrm{prob}(t) = \exp(-T(t)) \frac{\mathrm{d}T}{\mathrm{d}t} = \exp(-T(t)) h(t)$$

For example, if the hazard is

$$h(t) = \frac{\kappa}{\lambda} \left(\frac{t}{\lambda} \right)^{\kappa - 1},$$

then

$$T(t) = \left(\frac{t}{\lambda} \right)^{\kappa}$$

the probability density becomes:

$$h(t) = \exp\left[- \left(\frac{t}{\lambda} \right)^{\kappa} \right] \frac{\kappa}{\lambda} \left(\frac{t}{\lambda} \right)^{\kappa - 1}.$$

This is of course the Weibull distribution with parameters κ and λ.