

# Probabilistic Agent Based Modelling: Mathematical foundations

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## Abstract

In order to do modelling well we need to do calibration, data assimilation and uncertainty quantification properly. All of these problems can be posed in terms of probabilistic inference. At present, tools to do probabilistic inference on ABMs are lacking. In this paper I develop a mathematical foundation for thinking about and working with probabilistic inference in ABMs.

## 1 Agent based dynamical systems

We introduce the concept of an *agent based dynamical system* which consists of a set of interacting *agents*. Each agent has a state and can exchange messages with other agents. At any given time,  $t$ , each agent has a propensity,  $r$ , to perform an action such that, in the infinitesimal slice of time,  $[t, t + dt]$ , there is a probability  $rdt$  that the agent acts. The only actions an agent can perform are: send a message, change its internal state, create a new agent or leave the system completely.

We would like to have a convenient way of specifying agent behaviours and calculating how those behaviours relate to the aggregate behaviour of the whole system. In order to do probabilistic inference we will require a way of working with probability distributions over the system (i.e. the joint state of all agents) and calculating the posterior distribution given observations of the system.

### 1.1 Single agent

We start with the simplest possible agent based dynamical system: a system with only one stateless agent. Even a system as simple as this will allow us to introduce a few key concepts. Suppose that at time  $t = 0$  the agent definitely exists and between time  $t$  and  $t + dt$  the agent

leaves the system with probability  $rdt$ . We now introduce a variable,  $z$ , to represent the state that the agent is in the system and represent the probabilistic state of the system as a polynomial in  $z$

$$S = c + pz$$

where  $p$  is the probability that  $z$  is the case (i.e. that the agent is in the system) and  $c = (1 - p)$  is the probability that the system is empty. So, at time  $t = 0$ ,  $S(0) = z$ . Now, we introduce an important concept, borrowed from quantum field theory, called the *annihilation* operator which acts on probabilistic states. In our case, we can define the annihilation operator as

$$a = \frac{\partial}{\partial z}$$

If we apply this operator to  $S(0)$  we get  $aS(0) = az = \frac{\partial z}{\partial z} = 1$ . So the annihilation operator transforms a state in which there is definitely one agent into a state which is definitely empty, i.e. the agent is annihilated. We'll see later how this generalises very nicely to the case of multiple agents.

Similarly, we define a *creation operator*:

$$a^\dagger = z$$

If we apply the creation operator to a state which is definitely empty,  $S = 1$ , we get  $a^\dagger S = z$  which represents a state which definitely has one agent.

Given the creation and annihilation operators, it will be useful to know the rate of change of a probabilistic state if an agent has a propensity,  $r$ , to create or annihilate itself. Given an empty state and an agent that is currently outside of the system that has a propensity,  $r$ , to enter the system, then in time slice  $[t, t + dt]$  there is a probability  $rdt$  that the state will switch from empty to having an agent in it. So in time  $dt$  the probability of the empty

state goes down by  $rdt$  and the probability of there being an agent goes up by  $dt$ . So the rate of change of the state is given by

$$H_{a^\dagger} = \frac{\partial}{\partial t} = (a^\dagger - 1)r$$

Similarly, for the annihilation operator. If we start with an agent in the system, the probability of there being an agent decreases by  $rdt$  while the probability of the state being empty increases by the same amount. We can achieve this with the operator

$$H_a = \frac{\partial}{\partial t} = (a - a^\dagger a)r$$

We'll call  $H_{a^\dagger}$  and  $H_a$  the *Hamiltonians* for their respective operators. Again, we'll see later that by choosing this form for the Hamiltonians we make things very elegant when we come to generalise to many agents.

Once we have the Hamiltonian for a system, the probabilistic dynamics of the system is completely defined by the equation

$$\frac{\partial S}{\partial t} = HS$$

which is the probabilistic dynamics' analogue of Schrödinger's equation. This equation has a very general solution

$$S(t) = e^{tH}S(0)$$

where the exponent of an operator is defined as

$$e^{tH} = \sum_{k=0}^{\infty} \frac{(tH)^k}{k!}$$

and eponentiation of an operator is just repeated application (taking care to respect the order of non-commutative operators).

Going back now to the agent that has propensity  $r$  to annihilate itself, the equation of motion is

$$\frac{\partial S}{\partial t} = H_a S = \left( \frac{\partial}{\partial z} - z \frac{\partial}{\partial z} \right) rS$$

Solving this for  $S(0) = z$  gives

$$\begin{aligned} S(t) &= e^{rt((1-z)\frac{\partial}{\partial z})} z \\ &= \sum_{k=0}^{\infty} \frac{\left( rt(1-z)\frac{\partial}{\partial z} \right)^k}{k!} z \\ &= \sum_{k=0}^{\infty} \frac{(-rt)^k \left( (z-1)\frac{\partial}{\partial z} \right)^k}{k!} z \end{aligned}$$

but since  $\frac{\partial^n}{\partial z^n} = 0$  for  $n > 1$

$$\left( (z-1)\frac{\partial}{\partial z} \right)^k = (z-1)\frac{\partial}{\partial z}$$

for  $k > 0$ , so

$$S(t) = 1 + \sum_{k=0}^{\infty} \frac{(-rt)^k}{k!} (z-1)$$

where the initial 1 accounts for the case when  $k = 0$ . We can now turn the sum back into an exponent to give

$$S(t) = (1 - e^{-rt}) + e^{-rt}z$$

So the probability that the agent exists reduces exponentially as time progresses. This is exactly what we would expect.

## 1.2 Many agents

We can now show how our operators extend very elegantly to systems with more than one agent. In this case, we represent the state that there are definitely  $n$  agents in the system as  $S = z^n$ . A probabilistic state is therefore represented by a polynomial

$$S = \sum_{n=0}^{\infty} p_n z^n$$

where  $p_n$  is the probability that there are  $n$  agents, and

$$\sum_{n=0}^{\infty} p_n = 1$$

By choosing this representation, we can see immediately that our creation operator works on definite states:

$$a^\dagger z^n = z^{n+1}$$

Even better, it works on probabilistic states too. For example, suppose there's a 0.5 probability that the state is empty and a 0.5 probability that there's one agent, so  $S = 0.5 + 0.5z$ . In this case

$$a^\dagger(0.5 + 0.5z) = 0.5z + 0.5z^2$$

So there's now an equal probability of there being either one or two agents, i.e. the operator simultaneously adds an agent to all possible states.

If we start with an empty system (i.e.  $S(0) = 1$ ) and add agents at a constant rate we'd expect the Hamiltonian to be given by

$$\frac{\partial S}{\partial t} = H_{a^\dagger} S = (a^\dagger - 1)rS$$

This can again be solved analytically:

$$S(t) = e^{tH} = e^{-rt(1-z)} = e^{-rt} e^{rtz}$$

$$= e^{-rt} \sum_k \frac{(rt)^k}{k!} z^k$$

so, the probability of there being  $k$  agents (i.e. the coefficient of the  $k^{th}$  power of  $z$ ) is

$$c_k = \frac{(rt)^k e^{-rt}}{k!}$$

which is just the Poisson distribution, as we would expect.

Now let's try the annihilation operator on  $S = 0.5z + 0.5z^2$ :

$$a(0.5z + 0.5z^2) = 0.5 + z$$

We don't get  $0.5 + 0.5z$  as you may have expected. Instead, for a polynomial  $S = \sum_n p_n z^n$  we get

$$a \sum_n p_n z^n = \sum_n n p_n z^{n-1}$$

This behaviour can be harnessed to make a very useful operator

$$N = a^\dagger a$$

which in quantum field theory is called the number operator because it multiplies the probability of each state by the number of agents in that state

$$a^\dagger a \sum_n p_n z^n = \sum_n n p_n z^n$$

We can now understand the Hamiltonian of the annihilation operator in a new light

$$H_a = (a - a^\dagger a)r = (a^{\dagger-1} - 1)Nr$$

where  $a^{\dagger-1} = z^{-1}$  is the inverse of the creation operator, which we'll call the agent-based annihilation operator. In this form, we can understand the  $a^{\dagger-1}$  term as the transition operator for a single agent's propensity. The number operator  $N$  has the effect of applying this operator to all the agents in the system, as if we'd executed a `foreach` loop in a computer program.

This works for any operator that represents the transition function for an agent's propensity. Because it's so useful, we'll define a higher order function which takes an agent action  $T$  and returns the Hamiltonian that applies this propensity to all agents in a probabilistic state

$$\mathcal{H}(T) = (T - 1)Nr$$

To illustrate this, suppose we start with  $n$  agents and each agent has a propensity,  $r$ , to annihilate itself. In pseudocode this may look something like

```
foreach(a in S) {
  if(random() < r*dt) delete(a)
}
```

We can create the Hamiltonian for this

$$\frac{\partial}{\partial t} = \mathcal{H}(a^{\dagger-1}) = (a^{\dagger-1} - 1)Nr$$

Expanding this gives

$$H = (a^{\dagger-1} - 1)a^\dagger ar = (a - a^\dagger a)r$$

which is exactly the Hamiltonian from the single agent case, but now we understand why it has this form and why it will also work in the case of many agents.

The only difference here is the boundary condition. Instead of  $S(0) = z$  as in the single agent case, we now have  $S(0) = z^n$ . The solution to this is

$$S(t) = \sum_m \binom{n}{m} e^{-rtm} (1 - e^{-rt})^{n-m} z^m$$

The coefficients of  $z$  (i.e. the probabilities that there are  $m$  agents) make up a Binomial distribution, which, again, is what we would expect.

The above examples, although very simple, demonstrate how we can define a Hamiltonian operator in terms of the behaviour of an agent, yet apply that operator to the state of a whole system to get the aggregate behaviour.

### 1.3 Agent states

So far, the agents haven't had any internal state. We'll start simple again by giving agents a binary state which can be either 0 or 1. We'll represent an agent in state 0 as  $z_0$  and an agent in state 1 as  $z_1$ . A state with  $n$  agents in state  $z_0$  and  $m$  agents in state  $z_1$  is represented as state  $S = z_0^n z_1^m$ . We define annihilation and creation operators for each state:

$$a_0 = \frac{\partial}{\partial z_0}$$

$$a_1 = \frac{\partial}{\partial z_1}$$

$$a_0^\dagger = z_0$$

and

$$a_1^\dagger = z_1$$

Similarly, we now have two number operators  $N_0 = a_0^\dagger a_0$  and  $N_1 = a_1^\dagger a_1$  and two foreach operators  $E_0(T) = (T - 1)N_0$  and  $E_1 = (T - 1)N_1$  which act only on the agents in state 0 and 1 respectively.

A change of state from  $x$  to  $y$  can be represented as an agent in state  $x$  annihilating itself while simultaneously creating a new agent in state  $y$ ,  $a_y^\dagger a_x^{\dagger-1} = z_y z_x^{-1}$ .

Let's illustrate this with a system of  $n$  agents who each have a propensity  $r$  to flip to the opposite state. In pseudocode we want something like

```

S0 = S
foreach(x in S0 suchthat S0.state(x)=0) {
  if(random() < r*dt) S.state(x) = 1
}
foreach(x in S0 suchthat S0.state(x)=1) {
  if(random() < r*dt) S.state(x) = 0
}

```

This can be expressed as a Hamiltonian

$$H = rE_0(z_1 z_0^{-1}) + rE_1(z_0 z_1^{-1})$$

expanding this gives

$$H = r \left( (z_1 - z_0) \frac{\partial}{\partial z_0} + (z_0 - z_1) \frac{\partial}{\partial z_1} \right)$$

If we suppose that at time  $t = 0$  all agents are in state  $z_1$   
then we can solve

$$S(t) =$$